

**Supporting Information for:**

**Community Resource for Innovation in Polymer Technology (CRIPT): A Scalable Polymer  
Material Data Structure**

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## WRITTEN OUT EXAMPLE OF THE DATA MODEL

The following contains the full data model representation for example from Figure 6 of the main manuscript (chemical synthesis of polystyrene made by the secBuLi initiated anionic polymerization of styrene).

<b>User</b>	<b>3</b>
<b>Group</b>	<b>3</b>
<b>Project</b>	<b>3</b>
<b>Collection</b>	<b>4</b>
<b>Experiment</b>	<b>4</b>
<b>Inventory</b>	<b>4</b>
<b>Materials</b>	<b>5</b>
<i>Nitrogen</i>	5
<i>Argon</i>	10
<i>Tetrahydrofuran</i>	14
<i>Toluene</i>	20
<i>Water</i>	25
<i>Methanol</i>	30
<i>Styrene</i>	34
<i>1-Butanol</i>	39
<i>Sec-Butyl Lithium</i>	43
<i>Sec-Butyl Lithium Solution</i>	45
<i>Poly(styrene)</i>	48
<i>Deuterated Chloroform</i>	51
<b>Process</b>	<b>55</b>
<b>Data</b>	<b>59</b>
<i><sup>1</sup>H Nuclear Magnetic Resonance Spectrum</i>	59
<i>Size Exclusion Chromatography Trace</i>	60
<b>File</b>	<b>60</b>
<i><sup>1</sup>H Nuclear Magnetic Resonance Spectrum</i>	60
<i>Size Exclusion Chromatography Trace</i>	61
<b>Reference</b>	<b>61</b>

## USER

```
{
  "url": "local://cript/user/2aaa30ea-2b13-4804-92cf-a939bac745ac/",
  "uid": "2aaa30ea-2b13-4804-92cf-a939bac745ac",
  "public": false,
  "created_at": "2022-09-08T13:48:09.469494",
  "updated_at": "2022-09-08T13:48:09.469494",
  "username": "Tim",
  "email": "tim@cript.edu",
  "orcid_id": "",
  "groups": [],
  "model_version": "0.4.3"
}
```

## GROUP

```
{
  "url": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "uid": "5a5a9fb2-44ca-41e7-931d-b544a9a02b86",
  "public": false,
  "created_at": "2022-09-08T13:48:09.470495",
  "updated_at": "2022-09-08T13:48:09.470495",
  "name": "SDK test group",
  "users": [],
  "model_version": "0.4.3"
}
```

## PROJECT

```
{
  "url": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "uid": "ef26f322-8e03-4655-9aca-a731b6e5ae36",
  "public": false,
  "created_at": "2022-09-08T13:48:09.470495",
  "updated_at": "2022-09-08T13:48:09.470495",
  "name": "SDK test project",
  "materials": [],
  "files": [],
  "collections": [],
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3"
}
```

## **COLLECTION**

```
{
  "url": "local://cript/collection/fa73f5c7-75c5-4b5e-9390-955aefa2854f/",
  "uid": "fa73f5c7-75c5-4b5e-9390-955aefa2854f",
  "public": false,
  "created_at": "2022-09-08T13:48:09.471494",
  "updated_at": "2022-09-08T13:48:10.326308",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "Tutorial Examples",
  "experiments": [
    "local://cript/inventory/551c3b02-0185-4d57-80ac-394ca697f800/"
  ],
  "inventories": [],
  "citations": [],
  "notes": null,
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3"
}
```

## **EXPERIMENT**

```
{
  "url": "local://cript/experiment/37422b5c-fa9e-4377-b3de-18ef3105f0f4/",
  "uid": "37422b5c-fa9e-4377-b3de-18ef3105f0f4",
  "public": false,
  "created_at": "2022-09-08T13:48:09.471494",
  "updated_at": "2022-09-08T13:48:09.471494",
  "collection": "local://cript/collection/fa73f5c7-75c5-4b5e-9390-955aefa2854f/",
  "name": "Anionic Polymerization of Styrene with SecBuLi",
  "funding": [],
  "processes": [],
  "data": [],
  "notes": null,
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3"
}
```

## **INVENTORY**

```
{
  "url": "local://cript/inventory/551c3b02-0185-4d57-80ac-394ca697f800/",
  "uid": "551c3b02-0185-4d57-80ac-394ca697f800",
  "public": false,
  "created_at": "2022-09-08T13:48:10.323309",
  "updated_at": "2022-09-08T13:48:10.323309",
  "collection": "local://cript/collection/fa73f5c7-75c5-4b5e-9390-955aefa2854f/",
}
```

```

"name": "Tutorial Materials",
"description": null,
"materials": [
  "local://cript/material/cf7d4d83-88d7-4a3a-9eec-5f707c806b3b/",
  "local://cript/material/f8f76b12-12f3-4bf2-880d-75f13535e994/",
  "local://cript/material/8ddb53c1-738e-4c11-81c1-0e1e4fb53e84/",
  "local://cript/material/922c134c-99fc-4aac-ab22-4796dd3c6381/",
  "local://cript/material/c46b68d8-b521-4851-b85e-632ad3d02e96/",
  "local://cript/material/63f071c2-c64a-4b71-a84b-8de5b5812f4c/",
  "local://cript/material/46077c6a-1657-4d14-a8e5-645be25af625/",
  "local://cript/material/b719064a-0ece-4990-a0eb-f0e0fffab1e3/",
  "local://cript/material/df9e5147-a5cc-49e1-b11a-23dcc7263d3c/",
  "local://cript/material/89a49359-bb0a-40ba-8b0e-c4fbc02c7907/",
  "local://cript/material/3bc36780-f200-4954-9d58-2108e30c83a9/"
],
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## MATERIALS

### Nitrogen

```

{
  "url": "local://cript/material/8ddb53c1-738e-4c11-81c1-0e1e4fb53e84/",
  "uid": "8ddb53c1-738e-4c11-81c1-0e1e4fb53e84",
  "public": false,
  "created_at": "2022-09-08T13:48:10.313309",
  "updated_at": "2022-09-08T13:48:10.313309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "nitrogen",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "nitrogen"
    },
    {
      "key": "names",
      "value": [
        "N2",
        "dinitrogen"
      ]
    },
    {
      "key": "cas",
      "value": "7727-37-9"
    }
  ],
}

```

```

    {
      "key": "smiles",
      "value": "N#N"
    },
    {
      "key": "chem_formula",
      "value": "N2"
    },
    {
      "key": "pubchem_cid",
      "value": 947
    },
    {
      "key": "inchi_key",
      "value": "IJGRMHOSHXDMSA-UHFFFAOYSA-N"
    }
  ],
  "components": [],
  "keywords": [],
  "process": null,
  "properties": [
    {
      "key": "phase",
      "unit": null,
      "value": "gas",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    },
    {
      "key": "color",
      "unit": null,
      "value": "colorless",
      "type": null,
      "method": null,

```

```

    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 28.014,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/l",
    "value": 1.25,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
  }

```

```

"conditions": [
  {
    "key": "temperature",
    "unit": "degC",
    "value": 4,
    "type": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "material": null,
    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  }
],
"data": null,
"citations": [],
"notes": null
},
{
  "key": "+temp_boiling",
  "unit": "K",
  "value": 77.355,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [
    {
      "key": "pressure",
      "unit": "atm",
      "value": 1,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    }
  ]
}

```



```

    }
  ],
  "data": null,
  "citations": [],
  "notes": null
},
{
  "key": "temp_melt",
  "unit": "K",
  "value": 63.23,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [
    {
      "key": "pressure",
      "unit": "bar",
      "value": 1,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    }
  ],
  "data": null,
  "citations": [],
  "notes": null
}
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## Argon

```
{
  "url": "local://cript/material/922c134c-99fc-4aac-ab22-4796dd3c6381/",
  "uid": "922c134c-99fc-4aac-ab22-4796dd3c6381",
  "public": false,
  "created_at": "2022-09-08T13:48:10.314309",
  "updated_at": "2022-09-08T13:48:10.314309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "Argon",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "argon"
    },
    {
      "key": "names",
      "value": [
        "Ar"
      ]
    },
    {
      "key": "cas",
      "value": "7440-37-1"
    },
    {
      "key": "smiles",
      "value": "Ar"
    },
    {
      "key": "chem_formula",
      "value": "Ar"
    },
    {
      "key": "pubchem_cid",
      "value": 23968
    },
    {
      "key": "inchi_key",
      "value": "XKRIFYHLGVUSROY-UHFFFAOYSA-N"
    }
  ],
  "components": [],
  "keywords": [],
  "process": null,
  "properties": [
    {
```

```

    "key": "phase",
    "unit": null,
    "value": "gas",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "color",
    "unit": null,
    "value": "colorless",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 39.95,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,

```

```

    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/l",
    "value": 1.784,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 0,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    {
      "key": "pressure",
      "unit": "bar",
      "value": 1,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,

```

```

        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "+temp_boiling",
    "unit": "K",
    "value": 87.3,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "pressure",
            "unit": "atm",
            "value": 1,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        }
    ],
    "data": null,
    "citations": [],
    "notes": null
},
{
    "key": "temp_melt",
    "unit": "K",

```

```

    "value": 83.81,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### **Tetrahydrofuran**

```

{
  "url": "local://cript/material/46077c6a-1657-4d14-a8e5-645be25af625/",
  "uid": "46077c6a-1657-4d14-a8e5-645be25af625",
  "public": false,
  "created_at": "2022-09-08T13:48:10.317328",
  "updated_at": "2022-09-08T13:48:10.317328",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "thf",
  "identifiers": [

```

```

{
  "key": "preferred_name",
  "value": "tetrahydrofuran"
},
{
  "key": "names",
  "value": [
    "oxolane",
    "1,4-epoxybutane",
    "oxacyclopentane",
    "THF",
    "butylene oxide",
    "cycлотetramethylene oxide"
  ]
},
{
  "key": "cas",
  "value": "109-99-9"
},
{
  "key": "smiles",
  "value": "C1CCOC1"
},
{
  "key": "chem_formula",
  "value": "C4H8O"
},
{
  "key": "pubchem_cid",
  "value": 8028
},
{
  "key": "inchi_key",
  "value": "WYURNTSHIVDZCO-UHFFFAOYSA-N"
}
],
"components": [],
"keywords": [],
"process": null,
"properties": [
  {
    "key": "phase",
    "unit": null,
    "value": "liquid",
    "type": null,
    "method": null,

```

```

    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "color",
    "unit": null,
    "value": "colorless",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 72.107,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,

```



```

    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 0.8876,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 20,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "+temp_boiling",
    "unit": "degC",
    "value": 66,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,

```

```

    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "atm",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "temp_melt",
    "unit": "degC",
    "value": -108,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,

```

```

        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "+solubility",
    "unit": "g/ml",
    "value": -1,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "temperature",
            "unit": "degC",
            "value": 20,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        },
        {
            "key": "+solvent",
            "unit": null,
            "value": null,
            "type": null,
            "uncertainty": null,

```

```

      "uncertainty_type": null,
      "material": "local://cript/material/cf7d4d83-88d7-4a3a-9eec-5f707c806b3b/",
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    }
  ],
  "data": null,
  "citations": [],
  "notes": null
}
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## Toluene

```

{
  "url": "local://cript/material/63f071c2-c64a-4b71-a84b-8de5b5812f4c/",
  "uid": "63f071c2-c64a-4b71-a84b-8de5b5812f4c",
  "public": false,
  "created_at": "2022-09-08T13:48:10.316309",
  "updated_at": "2022-09-08T13:48:10.316309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "toluene",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "toluene"
    },
    {
      "key": "names",
      "value": [
        "methylbenzene"
      ]
    },
    {
      "key": "cas",
      "value": "108-88-3"
    },
    {
      "key": "smiles",
      "value": "Cc1ccccc1"
    }
  ],

```

```

    {
      "key": "chem_formula",
      "value": "C7H8"
    },
    {
      "key": "pubchem_cid",
      "value": 1140
    },
    {
      "key": "inchi_key",
      "value": "YXFVVABEGXRONW-UHFFFAOYSA-N"
    }
  ],
  "components": [],
  "keywords": [],
  "process": null,
  "properties": [
    {
      "key": "phase",
      "unit": null,
      "value": "liquid",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    },
    {
      "key": "color",
      "unit": null,
      "value": "colorless",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,

```

```

    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 92.141,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 0.87,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",

```

```

        "value": 25,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "+temp_boiling",
    "unit": "degC",
    "value": 111,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "pressure",
            "unit": "atm",
            "value": 1,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        }
    ]
},
"data": null,
"citations": [],

```

```

    "notes": null
  },
  {
    "key": "temp_melt",
    "unit": "degC",
    "value": -95,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "solubility",
    "unit": "g/L",
    "value": 0.52,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],

```



```

    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 20,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## Water

```

{
  "url": "local://cript/material/cf7d4d83-88d7-4a3a-9eec-5f707c806b3b/",
  "uid": "cf7d4d83-88d7-4a3a-9eec-5f707c806b3b",
  "public": false,
  "created_at": "2022-09-08T13:48:10.311309",
  "updated_at": "2022-09-08T13:48:10.311309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "water",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "water"
    },
    {
      "key": "names",
      "value": [
        "h2o",

```

```

        "dihydrogen oxide"
    ]
},
{
    "key": "cas",
    "value": "7732-18-5"
},
{
    "key": "smiles",
    "value": "O"
},
{
    "key": "chem_formula",
    "value": "H2O"
},
{
    "key": "pubchem_cid",
    "value": 962
},
{
    "key": "inchi_key",
    "value": "XLYOFNOQVPJJNP-UHFFFAOYSA-N"
}
],
"components": [],
"keywords": [],
"process": null,
"properties": [
    {
        "key": "phase",
        "unit": null,
        "value": "liquid",
        "type": null,
        "method": null,
        "method_description": null,
        "sample_preparation": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "components": [],
        "components_relative": [],
        "structure": null,
        "set_id": null,
        "conditions": [],
        "data": null,
        "citations": [],
        "notes": null
    }
]

```

```

},
{
  "key": "color",
  "unit": null,
  "value": "colorless",
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [],
  "data": null,
  "citations": [],
  "notes": null
},
{
  "key": "molar_mass",
  "unit": "g/mol",
  "value": 18.015,
  "type": null,
  "method": "prescribed",
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [],
  "data": null,
  "citations": [],
  "notes": null
},
{
  "key": "density",
  "unit": "g/ml",
  "value": 1.0,
  "type": null,
  "method": null,
  "method_description": null,

```

```

"sample_preparation": null,
"uncertainty": null,
"uncertainty_type": null,
"components": [],
"components_relative": [],
"structure": null,
"set_id": null,
"conditions": [
  {
    "key": "temperature",
    "unit": "degC",
    "value": 4,
    "type": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "material": null,
    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  }
],
"data": null,
"citations": [],
"notes": null
},
{
  "key": "+temp_boiling",
  "unit": "degC",
  "value": 100,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [
    {
      "key": "pressure",
      "unit": "atm",
      "value": 1,
      "type": null,

```

```

        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "temp_melt",
    "unit": "degC",
    "value": 0,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "pressure",
            "unit": "bar",
            "value": 1,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        }
    ],
    "data": null,
    "citations": [],
    "notes": null
}

```

```

],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## Methanol

```

{
  "url": "local://cript/material/df9e5147-a5cc-49e1-b11a-23dcc7263d3c/",
  "uid": "df9e5147-a5cc-49e1-b11a-23dcc7263d3c",
  "public": false,
  "created_at": "2022-09-08T13:48:10.320309",
  "updated_at": "2022-09-08T13:48:10.320309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "methanol",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "methanol"
    },
    {
      "key": "names",
      "value": [
        "Methyl alcohol",
        "CH3OH",
        "MeOH"
      ]
    },
    {
      "key": "cas",
      "value": "67-56-1"
    },
    {
      "key": "smiles",
      "value": "CO"
    },
    {
      "key": "chem_formula",
      "value": "CH4O"
    },
    {
      "key": "pubchem_cid",
      "value": 887
    },
    {
      "key": "inchi_key",

```

```

    "value": "OKKJLVBELUTLKV-UHFFFAOYSA-N"
  }
],
"components": [],
"keywords": [],
"process": null,
"properties": [
  {
    "key": "phase",
    "unit": null,
    "value": "liquid",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "color",
    "unit": null,
    "value": "colorless",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {

```

```

    "key": "molar_mass",
    "unit": "g/mol",
    "value": 32.0,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 0.792,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 20,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ]
  }

```



```

],
"data": null,
"citations": [],
"notes": null
},
{
  "key": "+temp_boiling",
  "unit": "degC",
  "value": 64.7,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [
    {
      "key": "pressure",
      "unit": "atm",
      "value": 1,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    }
  ],
  "data": null,
  "citations": [],
  "notes": null
},
{
  "key": "temp_melt",
  "unit": "degC",
  "value": -97.6,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,

```

```

    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## Styrene

```

{
  "url": "local://cript/material/c46b68d8-b521-4851-b85e-632ad3d02e96/",
  "uid": "c46b68d8-b521-4851-b85e-632ad3d02e96",
  "public": false,
  "created_at": "2022-09-08T13:48:10.315309",
  "updated_at": "2022-09-08T13:48:10.315309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "styrene",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "styrene"
    },
    {

```

```

    "key": "names",
    "value": [
      "vinylbenzene",
      "phenylethylene",
      "ethenylbenzene"
    ]
  },
  {
    "key": "cas",
    "value": "100-42-5"
  },
  {
    "key": "smiles",
    "value": "C=Cc1ccccc1"
  },
  {
    "key": "chem_formula",
    "value": "C8H8"
  },
  {
    "key": "pubchem_cid",
    "value": 7501
  },
  {
    "key": "inchi_key",
    "value": "PPBRXRYQALVLMV-UHFFFAOYSA-N"
  }
],
"components": [],
"keywords": [
  "styrene"
],
"process": null,
"properties": [
  {
    "key": "phase",
    "unit": null,
    "value": "liquid",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],

```

```

    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "color",
    "unit": null,
    "value": "colorless",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 104.15,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {

```

```

    "key": "density",
    "unit": "g/ml",
    "value": 0.906,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 25,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "+temp_boiling",
    "unit": "degC",
    "value": 145,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,

```

```

"conditions": [
  {
    "key": "pressure",
    "unit": "atm",
    "value": 1,
    "type": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "material": null,
    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  }
],
"data": null,
"citations": [],
"notes": null
},
{
  "key": "temp_melt",
  "unit": "degC",
  "value": -30,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [],
  "components_relative": [],
  "structure": null,
  "set_id": null,
  "conditions": [
    {
      "key": "pressure",
      "unit": "bar",
      "value": 1,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    }
  ]
}

```

```

    }
  ],
  "data": null,
  "citations": [],
  "notes": null
}
],
"notes": null,
"model_version": "0.4.3"
}

```

## 1-Butanol

```

{
  "url": "local://cript/material/b719064a-0ece-4990-a0eb-f0e0fffab1e3/",
  "uid": "b719064a-0ece-4990-a0eb-f0e0fffab1e3",
  "public": false,
  "created_at": "2022-09-08T13:48:10.319308",
  "updated_at": "2022-09-08T13:48:10.319308",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "nbutanol",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "1-butanol"
    },
    {
      "key": "names",
      "value": [
        "n-butanol",
        "n-butyl alcohol",
        "1-butyl alcohol",
        "nBuOH"
      ]
    },
    {
      "key": "cas",
      "value": "71-36-3"
    },
    {
      "key": "smiles",
      "value": "OCCCC"
    },
    {
      "key": "chem_formula",
      "value": "C4H10O"
    }
  ],

```

```

    {
      "key": "pubchem_cid",
      "value": 263
    },
    {
      "key": "inchi_key",
      "value": "LRHPLDYGYMQRHN-UHFFFAOYSA-N"
    }
  ],
  "components": [],
  "keywords": [],
  "process": null,
  "properties": [
    {
      "key": "phase",
      "unit": null,
      "value": "liquid",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    },
    {
      "key": "color",
      "unit": null,
      "value": "colorless",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,

```



```

    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 74.123,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 0.81,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 20,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,

```

```

        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "+temp_boiling",
    "unit": "degC",
    "value": 117.7,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "pressure",
            "unit": "atm",
            "value": 1,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        }
    ],
    "data": null,
    "citations": [],
    "notes": null
},
{
    "key": "temp_melt",

```

```

    "unit": "degC",
    "value": -89.9,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### Sec-Butyl Lithium

```

{
  "url": "local://cript/material/89a49359-bb0a-40ba-8b0e-c4fbc02c7907/",
  "uid": "89a49359-bb0a-40ba-8b0e-c4fbc02c7907",
  "public": false,
  "created_at": "2022-09-08T13:48:10.321309",
  "updated_at": "2022-09-08T13:48:10.321309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "secBuLi",

```

```

"identifiers": [
  {
    "key": "preferred_name",
    "value": "sec-butyllithium"
  },
  {
    "key": "names",
    "value": [
      "butan-2-yl lithium",
      "sBuLi",
      "secBuLi",
      "s-butyllithium"
    ]
  },
  {
    "key": "cas",
    "value": "598-30-1"
  },
  {
    "key": "smiles",
    "value": "[Li]C(C)CC"
  },
  {
    "key": "chem_formula",
    "value": "C4H9Li"
  },
  {
    "key": "pubchem_cid",
    "value": 887
  },
  {
    "key": "inchi_key",
    "value": "VATDYQWILMGLEW-UHFFFAOYSA-N"
  }
],
"components": [],
"keywords": [],
"process": null,
"properties": [
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 64.06,
    "type": null,
    "method": "prescribed",
    "method_description": null,
  }
]

```

```

    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### Sec-Butyl Lithium Solution

```

{
  "url": "local://cript/material/3bc36780-f200-4954-9d58-2108e30c83a9/",
  "uid": "3bc36780-f200-4954-9d58-2108e30c83a9",
  "public": false,
  "created_at": "2022-09-08T13:48:10.322309",
  "updated_at": "2022-09-08T13:48:10.322309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "SecBuLi solution 1.4M cHex",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "sec-butyllithium"
    },
    {
      "key": "names",
      "value": [
        "butan-2-yl lithium",
        "sBuLi",
        "secBuLi",
        "s-butyllithium"
      ]
    },
    {
      "key": "cas",
      "value": "598-30-1"
    },
    {

```

```

    "key": "smiles",
    "value": "[Li]C(C)CC"
  },
  {
    "key": "chem_formula",
    "value": "C4H9Li"
  },
  {
    "key": "pubchem_cid",
    "value": 887
  },
  {
    "key": "inchi_key",
    "value": "VATDYQWILMGLEW-UHFFFAOYSA-N"
  }
],
"components": [
  "local://cript/material/89a49359-bb0a-40ba-8b0e-c4fbc02c7907/",
  "local://cript/material/63f071c2-c64a-4b71-a84b-8de5b5812f4c/"
],
"keywords": [],
"process": null,
"properties": [
  {
    "key": "phase",
    "unit": null,
    "value": "solution",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 0.769,

```

```

"type": null,
"method": null,
"method_description": null,
"sample_preparation": null,
"uncertainty": null,
"uncertainty_type": null,
"components": [],
"components_relative": [],
"structure": null,
"set_id": null,
"conditions": [
  {
    "key": "pressure",
    "unit": "bar",
    "value": 1,
    "type": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "material": null,
    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  }
],
"data": null,
"citations": [],
"notes": null
},
{
  "key": "conc_molar",
  "unit": "M",
  "value": 1.4,
  "type": null,
  "method": null,
  "method_description": null,
  "sample_preparation": null,
  "uncertainty": null,
  "uncertainty_type": null,
  "components": [
    "local://cript/material/89a49359-bb0a-40ba-8b0e-c4fbc02c7907/"
  ],
  "components_relative": [
    "local://cript/material/63f071c2-c64a-4b71-a84b-8de5b5812f4c/"
  ],
  "structure": null,

```

```

      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    }
  ],
  "notes": null,
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3"
}

```

### **Poly(styrene)**

```

{
  "url": "local://cript/material/ea94529-623a-4e43-a094-4205fc7bb909/",
  "uid": "ea94529-623a-4e43-a094-4205fc7bb909",
  "public": false,
  "created_at": "2022-09-08T13:48:10.489312",
  "updated_at": "2022-09-08T13:48:10.489312",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "polystyrene",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "polystyrene"
    },
    {
      "key": "names",
      "value": [
        "poly(styrene)",
        "poly(vinylbenzene)"
      ]
    },
    {
      "key": "chem_repeat",
      "value": "C8H8"
    },
    {
      "key": "bigsmiles",
      "value": "[H]{}[>][<]C(C[>])c1ccccc1[<]}C(C)CC"
    },
    {
      "key": "cas",
      "value": "100-42-5"
    }
  ],
}

```



```

"components": [],
"keywords": [],
"process": "local://cript/process/ea11ef0e-cb4c-4ecb-91f1-ca7674ab103a/",
"properties": [
  {
    "key": "phase",
    "unit": null,
    "value": "solid",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "color",
    "unit": null,
    "value": "white",
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "mw_n",
    "unit": "g/mol",
    "value": 4800,

```

```

    "type": null,
    "method": "nmr",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": 400,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": "local://cript/data/b9d05e72-b095-467f-9853-42bb9284ae46/",
    "citations": [],
    "notes": null
  },
  {
    "key": "mw_n",
    "unit": "g/mol",
    "value": 5200,
    "type": null,
    "method": "sec",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": 100,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": "local://cript/data/b767d542-d319-4040-a028-934f099441e9/",
    "citations": [],
    "notes": null
  },
  {
    "key": "mw_d",
    "unit": null,
    "value": 1.03,
    "type": null,
    "method": "sec",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": 0.02,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],

```

```

    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": "local://cript/data/b767d542-d319-4040-a028-934f099441e9/",
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### Deuterated Chloroform

```

{
  "url": "local://cript/material/f8f76b12-12f3-4bf2-880d-75f13535e994/",
  "uid": "f8f76b12-12f3-4bf2-880d-75f13535e994",
  "public": false,
  "created_at": "2022-09-08T13:48:10.312309",
  "updated_at": "2022-09-08T13:48:10.312309",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "name": "deuterated chloroform",
  "identifiers": [
    {
      "key": "preferred_name",
      "value": "deuterated chloroform"
    },
    {
      "key": "names",
      "value": [
        "chloroform-d",
        "deuteriochloroform",
        "trichloro(deuterio)methane"
      ]
    },
    {
      "key": "cas",
      "value": "865-49-6"
    },
    {
      "key": "smiles",
      "value": "[2H]C(Cl)(Cl)Cl"
    },
    {
      "key": "chem_formula",
      "value": "CDCl3"
    }
  ]
}

```

```

    },
    {
      "key": "pubchem_cid",
      "value": 71583
    },
    {
      "key": "inchi_key",
      "value": "HEDRZPFGACZZDS-MICDWDOJSA-N"
    }
  ],
  "components": [],
  "keywords": [],
  "process": null,
  "properties": [
    {
      "key": "phase",
      "unit": null,
      "value": "liquid",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    },
    {
      "key": "color",
      "unit": null,
      "value": "colorless",
      "type": null,
      "method": null,
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "components": [],
      "components_relative": [],
      "structure": null,

```

```

    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "molar_mass",
    "unit": "g/mol",
    "value": 120.384,
    "type": null,
    "method": "prescribed",
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [],
    "data": null,
    "citations": [],
    "notes": null
  },
  {
    "key": "density",
    "unit": "g/ml",
    "value": 1.5,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "temperature",
        "unit": "degC",
        "value": 25,
        "type": null,
        "uncertainty": null,

```

```

        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
    }
],
"data": null,
"citations": [],
"notes": null
},
{
    "key": "+temp_boiling",
    "unit": "degC",
    "value": 61,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
        {
            "key": "pressure",
            "unit": "atm",
            "value": 1,
            "type": null,
            "uncertainty": null,
            "uncertainty_type": null,
            "material": null,
            "descriptor": null,
            "set_id": null,
            "measurement_id": null,
            "data": null
        }
    ],
    "data": null,
    "citations": [],
    "notes": null
},
{

```

```

    "key": "temp_melt",
    "unit": "degC",
    "value": -64,
    "type": null,
    "method": null,
    "method_description": null,
    "sample_preparation": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "components": [],
    "components_relative": [],
    "structure": null,
    "set_id": null,
    "conditions": [
      {
        "key": "pressure",
        "unit": "bar",
        "value": 1,
        "type": null,
        "uncertainty": null,
        "uncertainty_type": null,
        "material": null,
        "descriptor": null,
        "set_id": null,
        "measurement_id": null,
        "data": null
      }
    ],
    "data": null,
    "citations": [],
    "notes": null
  }
],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## PROCESS

```

{
  "url": "local://cript/process/ea11ef0e-cb4c-4ecb-91f1-ca7674ab103a/",
  "uid": "ea11ef0e-cb4c-4ecb-91f1-ca7674ab103a",
  "public": false,
  "created_at": "2022-09-08T13:48:10.407365",
  "updated_at": "2022-09-08T13:48:10.407365",
  "experiment": "local://cript/experiment/37422b5c-fa9e-4377-b3de-18ef3105f0f4/",

```

```

"name": "Anionic of Styrene",
"type": "multistep",
"keywords": [
  "polymerization",
  "living_poly",
  "anionic",
  "solution"
],
"description": "In an argon filled glovebox, a round bottom flask was filled with 216 ml of dried toluene. The solution of secBuLi (3 ml, 3.9 mmol) was added next, followed by styrene (22.3 g, 176 mmol) to initiate the polymerization. The reaction mixture immediately turned orange. After 30 min, the reaction was quenched with the addition of 3 ml of methanol. The polymer was isolated by precipitation in methanol 3 times and dried under vacuum.",
"prerequisite_processes": [],
"ingredients": [
  {
    "material": "local://cript/material/3bc36780-f200-4954-9d58-2108e30c83a9/",
    "keyword": "initiator",
    "quantities": [
      {
        "key": "volume",
        "unit": "ml",
        "value": 1,
        "uncertainty": null,
        "uncertainty_type": null
      }
    ]
  },
  {
    "material": "local://cript/material/63f071c2-c64a-4b71-a84b-8de5b5812f4c/",
    "keyword": "solvent",
    "quantities": [
      {
        "key": "volume",
        "unit": "ml",
        "value": 10,
        "uncertainty": null,
        "uncertainty_type": null
      }
    ]
  },
  {
    "material": "local://cript/material/c46b68d8-b521-4851-b85e-632ad3d02e96/",
    "keyword": "monomer",
    "quantities": [
      {

```



```

        "key": "mass",
        "unit": "g",
        "value": 0.455,
        "uncertainty": null,
        "uncertainty_type": null
    }
]
},
{
    "material": "local://cript/material/df9e5147-a5cc-49e1-b11a-23dcc7263d3c/",
    "keyword": "workup",
    "quantities": [
        {
            "key": "volume",
            "unit": "ml",
            "value": 0.1,
            "uncertainty": null,
            "uncertainty_type": null
        }
    ]
},
{
    "material": "local://cript/material/df9e5147-a5cc-49e1-b11a-23dcc7263d3c/",
    "keyword": "workup",
    "quantities": [
        {
            "key": "volume",
            "unit": "ml",
            "value": 0.1,
            "uncertainty": null,
            "uncertainty_type": null
        }
    ]
},
{
    "material": "local://cript/material/df9e5147-a5cc-49e1-b11a-23dcc7263d3c/",
    "keyword": "quench",
    "quantities": [
        {
            "key": "volume",
            "unit": "ml",
            "value": 100,
            "uncertainty": null,
            "uncertainty_type": null
        }
    ]
}
]

```

```

    }
  ],
  "equipment": [],
  "properties": [
    {
      "key": "yield_mass",
      "unit": "g",
      "value": 0.47,
      "type": null,
      "method": "scale",
      "method_description": null,
      "sample_preparation": null,
      "uncertainty": 0.02,
      "uncertainty_type": "stdev",
      "components": [],
      "components_relative": [],
      "structure": null,
      "set_id": null,
      "conditions": [],
      "data": null,
      "citations": [],
      "notes": null
    }
  ],
  "conditions": [
    {
      "key": "temperature",
      "unit": "degC",
      "value": 25,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,
      "descriptor": null,
      "set_id": null,
      "measurement_id": null,
      "data": null
    },
    {
      "key": "time_duration",
      "unit": "min",
      "value": 60,
      "type": null,
      "uncertainty": null,
      "uncertainty_type": null,
      "material": null,

```

```

    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  },
  {
    "key": "atm",
    "unit": null,
    "value": "none",
    "type": null,
    "uncertainty": null,
    "uncertainty_type": null,
    "material": "local://cript/material/922c134c-99fc-4aac-ab22-4796dd3c6381/",
    "descriptor": null,
    "set_id": null,
    "measurement_id": null,
    "data": null
  }
],
"set_id": null,
"products": [],
"waste": [],
"citations": [
  {
    "reference": "local://cript/reference/c8f4cd85-b717-4945-b862-319d37930705/",
    "type": "reference",
    "notes": null
  }
],
"citations": [],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

## DATA

### <sup>1</sup>H Nuclear Magnetic Resonance Spectrum

```

{
  "url": "local://cript/data/b9d05e72-b095-467f-9853-42bb9284ae46/",
  "uid": "b9d05e72-b095-467f-9853-42bb9284ae46",
  "public": false,
  "created_at": "2022-09-08T13:48:10.426312",
  "updated_at": "2022-09-08T13:48:10.426312",
  "experiment": "local://cript/experiment/37422b5c-fa9e-4377-b3de-18ef3105f0f4/",
  "name": "Crude 1H NMR of polystyrene",

```

```

"files": null,
"type": "nmr_h1",
"sample_preparation": null,
"calibration": null,
"configuration": null,
"materials": [],
"processes": [],
"citations": [],
"notes": null,
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### Size Exclusion Chromatography Trace

```

{
  "url": "local://cript/data/b767d542-d319-4040-a028-934f099441e9/",
  "uid": "b767d542-d319-4040-a028-934f099441e9",
  "public": false,
  "created_at": "2022-09-08T13:48:10.414384",
  "updated_at": "2022-09-08T13:48:10.434304",
  "experiment": "local://cript/experiment/37422b5c-fa9e-4377-b3de-18ef3105f0f4/",
  "name": "Crude SEC of polystyrene",
  "files": null,
  "type": "sec_trace",
  "sample_preparation": null,
  "calibration": null,
  "configuration": null,
  "materials": [],
  "processes": [],
  "citations": [],
  "notes": null,
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3",
  "file": [
    "local://cript/file/235bead1-2729-46a8-a5ea-d9b852b72c76/"
  ]
}

```

### FILE

#### <sup>1</sup>H Nuclear Magnetic Resonance Spectrum

```

{
  "url": "local://cript/file/235bead1-2729-46a8-a5ea-d9b852b72c76/",
  "uid": "235bead1-2729-46a8-a5ea-d9b852b72c76",
  "public": false,
  "created_at": "2022-09-08T13:48:10.431312",

```

```

"updated_at": "2022-09-08T13:48:10.431312",
"project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
"data": [
  "local://cript/data/b9d05e72-b095-467f-9853-42bb9284ae46/"
],
"type": "data",
"name": "nmr.txt",
"checksum": "f30de031a83357db695b3723d91c8ecfbaf9d9132b53b91811e35867365a35ce",
"unique_name": null,
"extension": ".txt",
"source": "C:/Users/nicep/Desktop/pyth_proj/cript/examples/test_data/nmr.txt",
"group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
"model_version": "0.4.3"
}

```

### Size Exclusion Chromatography Trace

```

{
  "url": "local://cript/file/ef2993c4-b687-4352-99cd-ac1280c5c0f6/",
  "uid": "ef2993c4-b687-4352-99cd-ac1280c5c0f6",
  "public": false,
  "created_at": "2022-09-08T13:48:10.418368",
  "updated_at": "2022-09-08T13:48:10.418368",
  "project": "local://cript/project/ef26f322-8e03-4655-9aca-a731b6e5ae36/",
  "data": [
    "local://cript/data/b767d542-d319-4040-a028-934f099441e9/"
  ],
  "type": "data",
  "name": "sec.txt",
  "checksum": "ec7a6e7598dc3c34cc954f461b132b71a8d43fd4b86752852c3ac187ac62cac7",
  "unique_name": null,
  "extension": ".txt",
  "source": "C:/Users/nicep/Desktop/pyth_proj/cript/examples/test_data/sec.txt",
  "group": "local://cript/group/5a5a9fb2-44ca-41e7-931d-b544a9a02b86/",
  "model_version": "0.4.3"
}

```

### REFERENCE

```

{
  "url": "local://cript/reference/c8f4cd85-b717-4945-b862-319d37930705/",
  "uid": "c8f4cd85-b717-4945-b862-319d37930705",
  "public": false,
  "created_at": "2022-09-12T17:47:11.083907",
  "updated_at": "2022-09-12T17:47:11.083907",
  "title": "Kinetics of Anionic Polymerization of Styrene in Tetrahydrofuran",
  "doi": "10.1021/ja00872a012",
}

```

```

"authors": [
  "Geacintov, C.",
  "Smid, J.",
  "Szwarc, M."
],
"journal": "Journal of the American Chemical Society",
"publisher": null,
"year": 1962,
"volume": 84,
"issue": 13,
"pages": [
  2508
],
"issn": null,
"arxiv_id": null,
"pmid": null,
"website": null,
"notes": null,
"group": "local://cript/group/875316df-1f7d-47ac-aa18-1030cf07d5c7/",
"model_version": "0.4.3"
}

```