# Saccharin

**Other names:**

1,1-Diox-1,2-benzisothiazol-3-one
1,1-Dioxide-1,2-benzisothiazol-3(2H)-one
1,1-Dioxido-3-oxo-2,3-dihydrobenzo[d]isothiazole
1,1-Dioxo-1,2-benzisothiazol-3(2H)-one
1,1-Dioxo-1,2-dihydro-benzo[d]isothiazol-3-one
1,2-Benzisothiazol-3(2H)-one, 1,1-dioxide
1,2-Benzisothiazolin-3-one, 1,1-dioxide
1,2-Benzisothiazoline-3-one 1,1-dioxide
1,2-Dihydro-2-ketobenzisosulfonazole
1,2-Dihydro-2-ketobenzisosulphonazole
1,2-benzisothiazol-3-one 1,1-dioxide
1,2-benzoisothiazolin-3-one 1,1-dioxide
2,3-Dihydro-1,2-benzisothiazol-3-one-1,1-dioxide
2,3-Dihydro-1,2-benzoisothiazol-3-one-1,1-dioxide
2,3-Dihydro-3-oxobenzisosulfonazole
2,3-Dihydro-3-oxobenzisosulphonazole
2-Sulfobenzoic acid imide
2-Sulfobenzoic imide
2-Sulphobenzoic imide
3-Benzisothiazolinone 1,1-dioxide
3-Hydroxybenzisothiazole S,S-dioxide
550 Saccharine
Anhydro-o-sulfaminebenzoic acid
Benzisosulfonazole, 2,3-dihydro-3-oxo-
Benzo-2-sulphimide
Benzo-sulphinide
Benzoic sulfimide
Benzoic sulphimide
Benzosulfimide
Benzosulfinide
Benzosulphimide
Benzoylsulfonic Imide
Garantose
Glucid
Gluside
Hermesetas
Insoluble saccharin
Kandiset
Natreen
RCRA Waste number U202

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|---|---|
| | Sacarina |
| | Saccharimide |
| | Saccharin acid |
| | Saccharin, insoluble |
| | Saccharina |
| | Saccharine |
| | Saccharinol |
| | Saccharinose |
| | Saccharol |
| | Sacharin |
| | Saxin |
| | Sucre edulcor |
| | Sucrette |
| | Sweeta |
| | Sykose |
| | Syncal |
| | Zaharina |
| | o-Benzoic acid sulfimide |
| | o-Benzoic sulfimide |
| | o-Benzoic sulphimide |
| | o-Benzosulfimide |
| | o-Benzosulphimide |
| | o-Benzoyl sulfimide |
| | o-Benzoyl sulphimide |
| | o-Sulfobenzimide |
| | o-Sulfobenzoic acid imide |
| **Inchi:** | InChI=1S/C7H5NO3S/c9-7-5-3-1-2-4-6(5)12(10,11)8-7/h1-4H,(H,8,9) |
| **InchiKey:** | CVHZOJJKTDOEJC-UHFFFAOYSA-N |
| **Formula:** | C7H5NO3S |
| **SMILES:** | O=C1NS(=O)(=O)c2ccccc21 |
| **Mol. weight [g/mol]:** | 183.18 |
| **CAS:** | 81-07-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -317.38 | kJ/mol | Joback Method |
| hf | -419.46 | kJ/mol | Joback Method |
| hfus | 24.61 | kJ/mol | Joback Method |
| hsub | 112.60 ± 4.20 | kJ/mol | NIST Webbook |

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|---|---|---|---|
| hvap | 62.97 | kJ/mol | Joback Method |
| log10ws | -1.64 | | Aqueous Solubility Prediction Method |
| logp | 0.119 | | Crippen Method |
| mcvol | 114.510 | ml/mol | McGowan Method |
| pc | 6729.65 | kPa | Joback Method |
| tb | 545.83 | K | Joback Method |
| tc | 785.52 | K | Joback Method |
| tf | 500.70 ± 1.50 | K | NIST Webbook |
| tf | 502.30 | K | Aqueous Solubility Prediction Method |
| tf | 499.00 ± 1.00 | K | NIST Webbook |
| tf | 501.00 ± 1.50 | K | NIST Webbook |
| tf | 500.75 ± 1.50 | K | NIST Webbook |
| tf | 498.40 ± 2.00 | K | NIST Webbook |
| tf | 499.45 | K | Determination and correlation of solubility and solution thermodynamics of saccharin in different pure solvents |
| vc | 0.440 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 245.40 | J/mol×K | 545.83 | Joback Method |
| cpg | 256.71 | J/mol×K | 585.78 | Joback Method |
| cpg | 267.26 | J/mol×K | 625.73 | Joback Method |
| cpg | 277.07 | J/mol×K | 665.67 | Joback Method |
| cpg | 286.14 | J/mol×K | 705.62 | Joback Method |
| cpg | 294.48 | J/mol×K | 745.57 | Joback Method |
| cpg | 302.11 | J/mol×K | 785.52 | Joback Method |
| hfust | 32.10 | kJ/mol | 502.90 | NIST Webbook |
| hfust | 26.77 | kJ/mol | 502.70 | NIST Webbook |
| hfust | 29.89 | kJ/mol | 500.70 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C81072&Units=SI

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Solid-liquid phase equilibrium and ternary phase diagrams of ethenzamide-saccharin cocrystals in different solvents:** | https://www.doi.org/10.1016/j.fluid.2016.02.047 |
| **Determination and correlation of solubility and solution thermodynamics of saccharin in different pure solvents:** | https://www.doi.org/10.1016/j.jct.2019.02.005 |
| **Solubility Determination for Carbamazepine and Saccharin in Methanol/Water Mixed Solvent: Basic Data for Design of Cocrystal Production by Antisolvent Crystallization:** | https://www.doi.org/10.1021/acs.jced.7b00920 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |