

3,5-Diiodosalicylaldehyde

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|-----------------------------|---|
| Other names: | Benzaldehyde, 2-hydroxy-3,5-diiodo- |
| Inchi: | InChI=1S/C7H4I2O2/c8-5-1-4(3-10)7(11)6(9)2-5/h1-3,11H |
| InchiKey: | MYWSBJKVOUZCIA-UHFFFAOYSA-N |
| Formula: | C7H4I2O2 |
| SMILES: | O=Cc1cc(I)cc(I)c1O |
| Mol. weight [g/mol]: | 373.91 |
| CAS: | 2631-77-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -36.69 | kJ/mol | Joback Method |
| hf | -83.37 | kJ/mol | Joback Method |
| hfus | 24.03 | kJ/mol | Joback Method |
| hvap | 73.26 | kJ/mol | Joback Method |
| log10ws | -3.56 | | Crippen Method |
| logp | 2.414 | | Crippen Method |
| mcvol | 144.810 | ml/mol | McGowan Method |
| pc | 5029.93 | kPa | Joback Method |
| tb | 711.76 | K | Joback Method |
| tc | 1008.66 | K | Joback Method |
| tf | 489.95 | K | Joback Method |
| vc | 0.478 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 255.36 | J/molxK | 711.76 | Joback Method |
| cpg | 261.18 | J/molxK | 761.24 | Joback Method |
| cpg | 266.62 | J/molxK | 810.73 | Joback Method |
| cpg | 271.89 | J/molxK | 860.21 | Joback Method |
| cpg | 277.15 | J/molxK | 909.69 | Joback Method |
| cpg | 282.62 | J/molxK | 959.17 | Joback Method |
| cpg | 288.46 | J/molxK | 1008.66 | Joback Method |
| dvisc | 0.0004535 | Paxs | 489.95 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002444 | Paxs | 526.92 | Joback Method |
| dvisc | 0.0001429 | Paxs | 563.89 | Joback Method |
| dvisc | 0.0000892 | Paxs | 600.86 | Joback Method |
| dvisc | 0.0000588 | Paxs | 637.82 | Joback Method |
| dvisc | 0.0000406 | Paxs | 674.79 | Joback Method |
| dvisc | 0.0000291 | Paxs | 711.76 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631778&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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

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