# Diallyl disulphide

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| **Other names:** | Allyl disulfide |
| | Diallyl disulfide |
| | Disulfide, di-2-propenyl |
| | Allyl disulphide |
| | 4,5-Dithia-1,7-octadiene |
| | 2-Propenyl disulphide |
| | di-2-Propenyl disulfide |
| | di-Propenyl disulfide |
| | dipropenyldisulfide (diallyl disulfide) |
| **Inchi:** | InChI=1S/C6H10S2/c1-3-5-7-8-6-4-2/h3-4H,1-2,5-6H2 |
| **InchiKey:** | PFRGXCVKLLPLIP-UHFFFAOYSA-N |
| **Formula:** | C6H10S2 |
| **SMILES:** | C=CCSSCC=C |
| **Mol. weight [g/mol]:** | 146.27 |
| **CAS:** | 2179-57-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 241.56 | kJ/mol | Joback Method |
| hf | 167.43 | kJ/mol | Joback Method |
| hfus | 17.00 | kJ/mol | Joback Method |
| hvap | 41.24 | kJ/mol | Joback Method |
| log10ws | -2.80 | | Crippen Method |
| logp | 2.740 | | Crippen Method |
| mcvol | 119.500 | ml/mol | McGowan Method |
| pc | 3560.02 | kPa | Joback Method |
| rinpol | 1082.00 | | NIST Webbook |
| rinpol | 1056.00 | | NIST Webbook |
| rinpol | 1085.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1064.00 | | NIST Webbook |
| rinpol | 1088.00 | | NIST Webbook |
| rinpol | 1083.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1085.00 | | NIST Webbook |
| rinpol | 1054.00 | | NIST Webbook |
| rinpol | 1048.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 1080.00 | NIST Webbook |
| rinpol | 1080.00 | NIST Webbook |
| rinpol | 1079.00 | NIST Webbook |
| rinpol | 1050.00 | NIST Webbook |
| rinpol | 1072.00 | NIST Webbook |
| rinpol | 1075.00 | NIST Webbook |
| rinpol | 1073.00 | NIST Webbook |
| rinpol | 1088.00 | NIST Webbook |
| rinpol | 1069.00 | NIST Webbook |
| rinpol | 1071.00 | NIST Webbook |
| rinpol | 1064.00 | NIST Webbook |
| rinpol | 1076.00 | NIST Webbook |
| rinpol | 1075.00 | NIST Webbook |
| rinpol | 1071.00 | NIST Webbook |
| rinpol | 1095.00 | NIST Webbook |
| rinpol | 1096.00 | NIST Webbook |
| rinpol | 1090.00 | NIST Webbook |
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| rinpol | 1065.00 | NIST Webbook |
| rinpol | 1073.00 | NIST Webbook |
| rinpol | 1087.00 | NIST Webbook |
| rinpol | 1077.00 | NIST Webbook |
| ripol | 1496.00 | NIST Webbook |
| ripol | 1526.00 | NIST Webbook |
| ripol | 1490.00 | NIST Webbook |
| ripol | 1480.00 | NIST Webbook |
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| ripol | 1475.00 | NIST Webbook |
| ripol | 1441.00 | NIST Webbook |
| ripol | 1490.00 | NIST Webbook |
| ripol | 1490.00 | NIST Webbook |
| ripol | 1463.00 | NIST Webbook |
| ripol | 1465.00 | NIST Webbook |
| ripol | 1465.00 | NIST Webbook |
| ripol | 1470.00 | NIST Webbook |
| ripol | 1480.00 | NIST Webbook |
| ripol | 1500.00 | NIST Webbook |
| ripol | 1475.00 | NIST Webbook |
| ripol | 1436.00 | NIST Webbook |
| ripol | 1436.00 | NIST Webbook |
| ripol | 1463.00 | NIST Webbook |
| ripol | 1468.00 | NIST Webbook |
| ripol | 1490.00 | NIST Webbook |
| ripol | 1490.00 | NIST Webbook |

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|---|---|---|---|
| tb | 460.70 | K | NIST Webbook |
| tc | 689.62 | K | Joback Method |
| tf | 222.66 | K | Joback Method |
| vc | 0.442 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 220.48 | J/mol×K | 467.60 | Joback Method |
| cpg | 231.22 | J/mol×K | 504.60 | Joback Method |
| cpg | 241.39 | J/mol×K | 541.61 | Joback Method |
| cpg | 251.01 | J/mol×K | 578.61 | Joback Method |
| cpg | 260.08 | J/mol×K | 615.62 | Joback Method |
| cpg | 268.62 | J/mol×K | 652.62 | Joback Method |
| cpg | 276.63 | J/mol×K | 689.62 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 352.20 | K | 2.10 | NIST Webbook |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179579&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |