

Diethyl disulphide

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| Other names: | 9,10-Dithiaoctadecane Bis(1-octyl) disulfide Diheptyl disulfide Diethyl disulfide Disulfide, diethyl Octyl disulfide di-n-Octyl disulfide n-Octyl disulfide |
| Inchi: | InChI=1S/C16H34S2/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3-16H2,1-2H3 |
| InchiKey: | AROCLDYPZXMJPW-UHFFFAOYSA-N |
| Formula: | C16H34S2 |
| SMILES: | CCCCCCCCSSCCCCCCCC |
| Mol. weight [g/mol]: | 290.57 |
| CAS: | 822-27-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 150.08 | kJ/mol | Joback Method |
| hf | -289.83 | kJ/mol | Joback Method |
| hfus | 45.46 | kJ/mol | Joback Method |
| hvap | 64.84 | kJ/mol | Joback Method |
| log10ws | -7.28 | | Crippen Method |
| logp | 7.089 | | Crippen Method |
| mcpvol | 269.000 | ml/mol | McGowan Method |
| pc | 1351.64 | kPa | Joback Method |
| tb | 703.04 | K | Joback Method |
| tc | 890.73 | K | Joback Method |
| tf | 338.88 | K | Joback Method |
| vc | 1.040 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 755.36 | J/mol×K | 703.04 | Joback Method |

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|-------|--------|---------|--------|---------------|
| cpg | 774.24 | J/mol×K | 734.32 | Joback Method |
| cpg | 792.15 | J/mol×K | 765.60 | Joback Method |
| cpg | 809.12 | J/mol×K | 796.89 | Joback Method |
| cpg | 825.17 | J/mol×K | 828.17 | Joback Method |
| cpg | 840.33 | J/mol×K | 859.45 | Joback Method |
| cpg | 854.61 | J/mol×K | 890.73 | Joback Method |
| hvapt | 73.90 | kJ/mol | 567.50 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.46108e+01 |
| Coeff. B | -5.12127e+03 |
| Coeff. C | -1.13276e+02 |
| Temperature range (K), min. | 470.83 |
| Temperature range (K), max. | 663.99 |

Sources

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|---|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C822275&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| 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 |

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 |

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|-----------------|---|
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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