# 2,2-Diphenyl-4-mercaptobutyric acid

**Inchi:** InChI=1S/C16H16O2S/c17-15(18)16(11-12-19,13-7-3-1-4-8-13)14-9-5-2-6-10-14/h1-10,1
**InchiKey:** ZWILEONEUTXNPU-UHFFFAOYSA-N
**Formula:** C16H16O2S
**SMILES:** O=C(O)C(CCS)(c1ccccc1)c1ccccc1
**Mol. weight [g/mol]:** 272.36
**CAS:** 73758-57-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.15 | kJ/mol | Joback Method |
| hf | -135.59 | kJ/mol | Joback Method |
| hfus | 27.59 | kJ/mol | Joback Method |
| hvap | 84.63 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 3.377 | | Crippen Method |
| mcvol | 212.570 | ml/mol | McGowan Method |
| pc | 2909.25 | kPa | Joback Method |
| tb | 824.52 | K | Joback Method |
| tc | 1068.34 | K | Joback Method |
| tf | 472.55 | K | Joback Method |
| vc | 0.783 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 596.03 | J/mol×K | 824.52 | Joback Method |
| cpg | 608.30 | J/mol×K | 865.16 | Joback Method |
| cpg | 619.53 | J/mol×K | 905.79 | Joback Method |
| cpg | 629.85 | J/mol×K | 946.43 | Joback Method |
| cpg | 639.38 | J/mol×K | 987.07 | Joback Method |
| cpg | 648.24 | J/mol×K | 1027.70 | Joback Method |
| cpg | 656.56 | J/mol×K | 1068.34 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C73758573&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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

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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 |
| **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 |