# Diethylmalonic acid, hexyl 2-methylthiophenyl ester

**Inchi:** InChI=1S/C20H30O4S/c1-5-8-9-12-15-23-18(21)20(6-2,7-3)19(22)24-16-13-10-11-14-17

**InchiKey:** HFVMHNPBSSOKQW-UHFFFAOYSA-N

**Formula:** C20H30O4S

**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC

**Mol. weight [g/mol]:** 366.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -211.58 | kJ/mol | Joback Method |
| hf | -687.55 | kJ/mol | Joback Method |
| hfus | 43.50 | kJ/mol | Joback Method |
| hvap | 86.88 | kJ/mol | Joback Method |
| log10ws | -5.75 | | Crippen Method |
| logp | 5.244 | | Crippen Method |
| mcvol | 300.130 | ml/mol | McGowan Method |
| pc | 1377.86 | kPa | Joback Method |
| rinpol | 2459.00 | | NIST Webbook |
| rinpol | 2459.00 | | NIST Webbook |
| tb | 906.79 | K | Joback Method |
| tc | 1125.12 | K | Joback Method |
| tf | 535.24 | K | Joback Method |
| vc | 1.139 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 937.34 | J/mol×K | 906.79 | Joback Method |
| cpg | 952.15 | J/mol×K | 943.18 | Joback Method |
| cpg | 965.65 | J/mol×K | 979.57 | Joback Method |
| cpg | 977.89 | J/mol×K | 1015.96 | Joback Method |
| cpg | 988.91 | J/mol×K | 1052.34 | Joback Method |
| cpg | 998.74 | J/mol×K | 1088.73 | Joback Method |
| cpg | 1007.44 | J/mol×K | 1125.12 | Joback Method |

# Sources

| | |
|---|---|
| **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=U369533&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |