

Dimethylmalonic acid, heptadecyl heptyl ester

Inchi: InChI=1S/C29H56O4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-22-24-26-33-28(31)29(3,4)27
InchiKey: XNKALXUDZOCIDM-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCC
Mol. weight [g/mol]: 468.75

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -271.70 | kJ/mol | Joback Method |
| hf | -1140.24 | kJ/mol | Joback Method |
| hfus | 69.03 | kJ/mol | Joback Method |
| hvap | 97.16 | kJ/mol | Joback Method |
| log10ws | -9.45 | | Crippen Method |
| logp | 8.941 | | Crippen Method |
| mvol | 434.350 | ml/mol | McGowan Method |
| pc | 660.51 | kPa | Joback Method |
| rinpol | 3010.00 | | NIST Webbook |
| rinpol | 3010.00 | | NIST Webbook |
| tb | 1012.27 | K | Joback Method |
| tc | 1256.59 | K | Joback Method |
| tf | 563.33 | K | Joback Method |
| vc | 1.696 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1539.29 | J/molxK | 1012.27 | Joback Method |
| cpg | 1562.26 | J/molxK | 1052.99 | Joback Method |
| cpg | 1583.28 | J/molxK | 1093.71 | Joback Method |
| cpg | 1602.46 | J/molxK | 1134.43 | Joback Method |
| cpg | 1619.92 | J/molxK | 1175.15 | Joback Method |
| cpg | 1635.76 | J/molxK | 1215.87 | Joback Method |
| cpg | 1650.11 | J/molxK | 1256.59 | Joback Method |
| dvisc | 0.0002393 | Paxs | 563.33 | Joback Method |

| | | | | |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001037 | Paxs | 638.15 | Joback Method |
| dvisc | 0.0000535 | Paxs | 712.98 | Joback Method |
| dvisc | 0.0000313 | Paxs | 787.80 | Joback Method |
| dvisc | 0.0000201 | Paxs | 862.62 | Joback Method |
| dvisc | 0.0000139 | Paxs | 937.45 | Joback Method |
| dvisc | 0.0000101 | Paxs | 1012.27 | Joback Method |

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=U361908&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| 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 |

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<https://www.chemeo.com/cid/45-947-1/Dimethylmalonic-acid-heptadecyl-heptyl-ester.pdf>

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