

Malonic acid, dodecyl 2-methylpentyl ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C21H40O4/c1-4-6-7-8-9-10-11-12-13-14-16-24-20(22)17-21(23)25-18-19(3)15 |
| InchiKey: | PSLDOKPWMTMJBRC-UHFFFAOYSA-N |
| Formula: | C21H40O4 |
| SMILES: | CCCCCCCCCCCCOC(=O)CC(=O)OCC(C)CCC |
| Mol. weight [g/mol]: | 356.54 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -344.34 | kJ/mol | Joback Method |
| hf | -971.65 | kJ/mol | Joback Method |
| hfus | 52.20 | kJ/mol | Joback Method |
| hvap | 80.26 | kJ/mol | Joback Method |
| log10ws | -6.10 | | Crippen Method |
| logp | 5.820 | | Crippen Method |
| mcvol | 321.630 | ml/mol | McGowan Method |
| pc | 1018.13 | kPa | Joback Method |
| rinpol | 2304.00 | | NIST Webbook |
| rinpol | 2304.00 | | NIST Webbook |
| tb | 832.02 | K | Joback Method |
| tc | 1019.80 | K | Joback Method |
| tf | 455.75 | K | Joback Method |
| vc | 1.254 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1030.73 | J/molxK | 832.02 | Joback Method |
| cpg | 1113.31 | J/molxK | 988.51 | Joback Method |
| cpg | 1098.97 | J/molxK | 957.21 | Joback Method |
| cpg | 1083.56 | J/molxK | 925.91 | Joback Method |
| cpg | 1067.07 | J/molxK | 894.61 | Joback Method |
| cpg | 1049.46 | J/molxK | 863.32 | Joback Method |
| cpg | 1126.61 | J/molxK | 1019.80 | Joback Method |
| dvisc | 0.0000422 | Paxs | 832.02 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000570 | Paxs | 769.31 | Joback Method |
| dvisc | 0.0000812 | Paxs | 706.60 | Joback Method |
| dvisc | 0.0001238 | Paxs | 643.88 | Joback Method |
| dvisc | 0.0002068 | Paxs | 581.17 | Joback Method |
| dvisc | 0.0003912 | Paxs | 518.46 | Joback Method |
| dvisc | 0.0008818 | Paxs | 455.75 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349304&Units=SI |

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/80-164-1/Malonic-acid-dodecyl-2-methylpentyl-ester.pdf>

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