

Malonic acid, 4-methylpent-2-yl tetradecyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C23H44O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-26-22(24)19-23(25)27-21(4) |
| InchiKey: | OUSZLVYQQAGDKQ-UHFFFAOYSA-N |
| Formula: | C23H44O4 |
| SMILES: | CCCCCCCCCCCCCOC(=O)CC(=O)OC(C)CC(C)C |
| Mol. weight [g/mol]: | 384.59 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -329.94 | kJ/mol | Joback Method |
| hf | -1018.21 | kJ/mol | Joback Method |
| hfus | 53.85 | kJ/mol | Joback Method |
| hvap | 84.33 | kJ/mol | Joback Method |
| log10ws | -7.05 | | Crippen Method |
| logp | 6.599 | | Crippen Method |
| mcvol | 349.810 | ml/mol | McGowan Method |
| pc | 908.34 | kPa | Joback Method |
| rinpol | 2481.00 | | NIST Webbook |
| rinpol | 2481.00 | | NIST Webbook |
| tb | 877.34 | K | Joback Method |
| tc | 1074.11 | K | Joback Method |
| tf | 463.29 | K | Joback Method |
| vc | 1.359 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1155.40 | J/molxK | 877.34 | Joback Method |
| cpg | 1240.52 | J/molxK | 1041.32 | Joback Method |
| cpg | 1226.01 | J/molxK | 1008.52 | Joback Method |
| cpg | 1210.26 | J/molxK | 975.73 | Joback Method |
| cpg | 1193.27 | J/molxK | 942.93 | Joback Method |
| cpg | 1174.99 | J/molxK | 910.14 | Joback Method |
| cpg | 1253.84 | J/molxK | 1074.11 | Joback Method |
| dvisc | 0.0000286 | Paxs | 877.34 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000394 | Paxs | 808.33 | Joback Method |
| dvisc | 0.0000577 | Paxs | 739.32 | Joback Method |
| dvisc | 0.0000911 | Paxs | 670.32 | Joback Method |
| dvisc | 0.0001600 | Paxs | 601.31 | Joback Method |
| dvisc | 0.0003252 | Paxs | 532.30 | Joback Method |
| dvisc | 0.0008160 | Paxs | 463.29 | 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=U349342&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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