

Glutaric acid, 2-methylpentyl tridecyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C24H46O4/c1-4-6-7-8-9-10-11-12-13-14-15-20-27-23(25)18-16-19-24(26)28-2 |
| InchiKey: | MUQVHINITGAAMSQ-UHFFFAOYSA-N |
| Formula: | C24H46O4 |
| SMILES: | CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(C)CC |
| Mol. weight [g/mol]: | 398.62 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -319.08 | kJ/mol | Joback Method |
| hf | -1033.57 | kJ/mol | Joback Method |
| hfus | 59.97 | kJ/mol | Joback Method |
| hvap | 86.94 | kJ/mol | Joback Method |
| log10ws | -7.35 | | Crippen Method |
| logp | 6.990 | | Crippen Method |
| mcvol | 363.900 | ml/mol | McGowan Method |
| pc | 853.96 | kPa | Joback Method |
| rinpola | 2763.00 | | NIST Webbook |
| tb | 900.66 | K | Joback Method |
| tc | 1103.57 | K | Joback Method |
| tf | 489.56 | K | Joback Method |
| vc | 1.421 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1218.00 | J/molxK | 900.66 | Joback Method |
| cpg | 1238.11 | J/molxK | 934.48 | Joback Method |
| cpg | 1256.81 | J/molxK | 968.30 | Joback Method |
| cpg | 1274.13 | J/molxK | 1002.12 | Joback Method |
| cpg | 1290.12 | J/molxK | 1035.94 | Joback Method |
| cpg | 1304.80 | J/molxK | 1069.75 | Joback Method |
| cpg | 1318.20 | J/molxK | 1103.57 | Joback Method |
| dvisc | 0.0006076 | Paxs | 489.56 | Joback Method |
| dvisc | 0.0002626 | Paxs | 558.08 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001364 | Paxs | 626.59 | Joback Method |
| dvisc | 0.0000806 | Paxs | 695.11 | Joback Method |
| dvisc | 0.0000523 | Paxs | 763.63 | Joback Method |
| dvisc | 0.0000365 | Paxs | 832.14 | Joback Method |
| dvisc | 0.0000269 | Paxs | 900.66 | 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=U358422&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/12-422-9/Glutaric-acid-2-methylpentyl-tridecyl-ester.pdf>

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