

Glutaric acid, 5-methoxy-3-methylpent-2-yl octyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C20H38O5/c1-5-6-7-8-9-10-15-24-19(21)12-11-13-20(22)25-18(3)17(2)14-16-2 |
| InchiKey: | MOHHARIJEATOLV-UHFFFAOYSA-N |
| Formula: | C20H38O5 |
| SMILES: | CCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)CCOC |
| Mol. weight [g/mol]: | 358.51 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -460.20 | kJ/mol | Joback Method |
| hf | -1088.51 | kJ/mol | Joback Method |
| hfus | 47.27 | kJ/mol | Joback Method |
| hvap | 80.06 | kJ/mol | Joback Method |
| log10ws | -4.88 | | Crippen Method |
| logp | 4.665 | | Crippen Method |
| mcvol | 313.410 | ml/mol | McGowan Method |
| pc | 1077.10 | kPa | Joback Method |
| rinpol | 2406.00 | | NIST Webbook |
| rinpol | 2406.00 | | NIST Webbook |
| tb | 831.12 | K | Joback Method |
| tc | 1019.53 | K | Joback Method |
| tf | 451.71 | K | Joback Method |
| vc | 1.210 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1001.80 | J/molxK | 831.12 | Joback Method |
| cpg | 1080.94 | J/molxK | 988.13 | Joback Method |
| cpg | 1067.40 | J/molxK | 956.73 | Joback Method |
| cpg | 1052.72 | J/molxK | 925.33 | Joback Method |
| cpg | 1036.90 | J/molxK | 893.92 | Joback Method |
| cpg | 1019.93 | J/molxK | 862.52 | Joback Method |
| cpg | 1093.35 | J/molxK | 1019.53 | Joback Method |
| dvisc | 0.0000335 | Paxs | 831.12 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000456 | Paxs | 767.88 | Joback Method |
| dvisc | 0.0000658 | Paxs | 704.65 | Joback Method |
| dvisc | 0.0001019 | Paxs | 641.41 | Joback Method |
| dvisc | 0.0001737 | Paxs | 578.18 | Joback Method |
| dvisc | 0.0003376 | Paxs | 514.95 | Joback Method |
| dvisc | 0.0007901 | Paxs | 451.71 | 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=U358437&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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