

Glutaric acid, 5-methoxy-3-phenylpentyl propyl ester

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| Inchi: | InChI=1S/C20H30O5/c1-3-14-24-19(21)10-7-11-20(22)25-16-13-18(12-15-23-2)17-8-5-4 |
| InchiKey: | JYMZUZJYEGZSOJ-UHFFFAOYSA-N |
| Formula: | C20H30O5 |
| SMILES: | CCCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1 |
| Mol. weight [g/mol]: | 350.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -345.35 | kJ/mol | Joback Method |
| hf | -846.70 | kJ/mol | Joback Method |
| hfus | 44.84 | kJ/mol | Joback Method |
| hvap | 82.72 | kJ/mol | Joback Method |
| log10ws | -4.07 | | Crippen Method |
| logp | 3.864 | | Crippen Method |
| mvol | 289.650 | ml/mol | McGowan Method |
| pc | 1347.68 | kPa | Joback Method |
| rinpol | 2506.00 | | NIST Webbook |
| rinpol | 2506.00 | | NIST Webbook |
| tb | 858.24 | K | Joback Method |
| tc | 1060.35 | K | Joback Method |
| tf | 493.13 | K | Joback Method |
| vc | 1.107 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 908.30 | J/molxK | 858.24 | Joback Method |
| cpg | 975.31 | J/molxK | 1026.67 | Joback Method |
| cpg | 964.31 | J/molxK | 992.98 | Joback Method |
| cpg | 952.12 | J/molxK | 959.30 | Joback Method |
| cpg | 938.74 | J/molxK | 925.61 | Joback Method |
| cpg | 924.14 | J/molxK | 891.93 | Joback Method |
| cpg | 985.15 | J/molxK | 1060.35 | Joback Method |
| dvisc | 0.0000371 | Paxs | 858.24 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000490 | Paxs | 797.39 | Joback Method |
| dvisc | 0.0000677 | Paxs | 736.54 | Joback Method |
| dvisc | 0.0000992 | Paxs | 675.68 | Joback Method |
| dvisc | 0.0001568 | Paxs | 614.83 | Joback Method |
| dvisc | 0.0002740 | Paxs | 553.98 | Joback Method |
| dvisc | 0.0005494 | Paxs | 493.13 | 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=U359528&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m_{cvol}: | 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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