

Glutaric acid, cyclohexylmethyl diphenylmethyl ester

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| Inchi: | InChI=1S/C25H30O4/c26-23(28-19-20-11-4-1-5-12-20)17-10-18-24(27)29-25(21-13-6-2- |
| InchiKey: | ITINOSZVSWAWSO-UHFFFAOYSA-N |
| Formula: | C25H30O4 |
| SMILES: | O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)OCC1CCCCC1 |
| Mol. weight [g/mol]: | 394.50 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -61.39 | kJ/mol | Joback Method |
| hf | -526.83 | kJ/mol | Joback Method |
| hfus | 42.47 | kJ/mol | Joback Method |
| hvap | 94.15 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 5.613 | | Crippen Method |
| mvol | 319.610 | ml/mol | McGowan Method |
| pc | 1422.92 | kPa | Joback Method |
| rinpol | 3046.00 | | NIST Webbook |
| rinpol | 3046.00 | | NIST Webbook |
| tb | 996.45 | K | Joback Method |
| tc | 1237.64 | K | Joback Method |
| tf | 561.05 | K | Joback Method |
| vc | 1.194 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1071.36 | J/molxK | 996.45 | Joback Method |
| cpg | 1085.73 | J/molxK | 1036.65 | Joback Method |
| cpg | 1098.34 | J/molxK | 1076.85 | Joback Method |
| cpg | 1109.29 | J/molxK | 1117.05 | Joback Method |
| cpg | 1118.65 | J/molxK | 1157.24 | Joback Method |
| cpg | 1126.50 | J/molxK | 1197.44 | Joback Method |
| cpg | 1132.95 | J/molxK | 1237.64 | Joback Method |
| dvisc | 0.0004220 | Paxs | 561.05 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002012 | Paxs | 633.62 | Joback Method |
| dvisc | 0.0001116 | Paxs | 706.18 | Joback Method |
| dvisc | 0.0000692 | Paxs | 778.75 | Joback Method |
| dvisc | 0.0000465 | Paxs | 851.32 | Joback Method |
| dvisc | 0.0000333 | Paxs | 923.88 | Joback Method |
| dvisc | 0.0000250 | Paxs | 996.45 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393347&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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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