

Glutaric acid, (2-methylcyclohex-1-enyl)methyl

InChI: 1S/C19H23FO4/c1-14-7-2-3-8-15(14)13-23-18(21)11-6-12-19(22)24-17-10-5-4-9-
InChIKey: FYZABUYBMPHNOS-UHFFFAOYSA-N

Formula: C19H23FO4

SMILES: CC1=C(COC(=O)CCCC(=O)Oc2ccccc2F)CCCC1

Mol. weight [g/mol]: 334.38

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -407.91 | kJ/mol | Joback Method |
| hf | -786.64 | kJ/mol | Joback Method |
| hfus | 38.48 | kJ/mol | Joback Method |
| hvap | 80.67 | kJ/mol | Joback Method |
| log10ws | -5.33 | | Crippen Method |
| logp | 4.335 | | Crippen Method |
| mcvol | 256.300 | ml/mol | McGowan Method |
| pc | 1686.56 | kPa | Joback Method |
| rinpol | 2419.00 | | NIST Webbook |
| tb | 850.97 | K | Joback Method |
| tc | 1068.23 | K | Joback Method |
| tf | 525.16 | K | Joback Method |
| vc | 0.978 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 787.46 | J/molxK | 850.97 | Joback Method |
| cpg | 802.49 | J/molxK | 887.18 | Joback Method |
| cpg | 816.22 | J/molxK | 923.39 | Joback Method |
| cpg | 828.69 | J/molxK | 959.60 | Joback Method |
| cpg | 839.92 | J/molxK | 995.81 | Joback Method |
| cpg | 849.92 | J/molxK | 1032.02 | Joback Method |
| cpg | 858.73 | J/molxK | 1068.23 | 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=U405505&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | 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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