# Glutaric acid, 2,5-difluorobenzyl 2-methylhex-3-yl ester

**Inchi:** InChI=1S/C19H26F2O4/c1-4-6-17(13(2)3)25-19(23)8-5-7-18(22)24-12-14-11-15(20)9-10

**InchiKey:** GISZEBLSOXPSBI-UHFFFAOYSA-N

**Formula:** C19H26F2O4

**SMILES:** CCCC(OC(=O)CCCC(=O)OCc1cc(F)ccc1F)C(C)C

**Mol. weight [g/mol]:** 356.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -660.09 | kJ/mol | Joback Method |
| hf | -1114.28 | kJ/mol | Joback Method |
| hfus | 42.92 | kJ/mol | Joback Method |
| hvap | 77.39 | kJ/mol | Joback Method |
| log10ws | -5.63 | | Crippen Method |
| logp | 4.546 | | Crippen Method |
| mcvol | 273.230 | ml/mol | McGowan Method |
| pc | 1348.67 | kPa | Joback Method |
| rinpol | 2202.00 | | NIST Webbook |
| rinpol | 2202.00 | | NIST Webbook |
| tb | 821.00 | K | Joback Method |
| tc | 1016.29 | K | Joback Method |
| tf | 470.85 | K | Joback Method |
| vc | 1.063 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 834.34 | J/mol×K | 821.00 | Joback Method |
| cpg | 849.57 | J/mol×K | 853.55 | Joback Method |
| cpg | 863.74 | J/mol×K | 886.10 | Joback Method |
| cpg | 876.86 | J/mol×K | 918.65 | Joback Method |
| cpg | 888.96 | J/mol×K | 951.20 | Joback Method |
| cpg | 900.04 | J/mol×K | 983.74 | Joback Method |
| cpg | 910.13 | J/mol×K | 1016.29 | Joback Method |

# Sources

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|---|---|
| **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=U376947&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **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 |