# Glutaric acid, di(2,5-difluorobenzyl) ester

**Inchi:** InChI=1S/C19H16F4O4/c20-14-4-6-16(22)12(8-14)10-26-18(24)2-1-3-19(25)27-11-13-9-15(21)5-7-17(13)23/h4-9H,1-3,10-11H2

**InchiKey:** MCRRIWGBIFJZCM-UHFFFAOYSA-N

**Formula:** C19H16F4O4

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

**Mol. weight [g/mol]:** 384.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -951.68 | kJ/mol | Joback Method |
| hf | -1282.35 | kJ/mol | Joback Method |
| hfus | 49.39 | kJ/mol | Joback Method |
| hvap | 80.13 | kJ/mol | Joback Method |
| log10ws | -6.02 | | Crippen Method |
| logp | 4.200 | | Crippen Method |
| mcvol | 253.010 | ml/mol | McGowan Method |
| pc | 1564.75 | kPa | Joback Method |
| rinpol | 2418.00 | | NIST Webbook |
| rinpol | 2418.00 | | NIST Webbook |
| tb | 857.06 | K | Joback Method |
| tc | 1062.03 | K | Joback Method |
| tf | 553.49 | K | Joback Method |
| vc | 1.004 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 750.40 | J/mol×K | 857.06 | Joback Method |
| cpg | 762.38 | J/mol×K | 891.22 | Joback Method |
| cpg | 773.32 | J/mol×K | 925.38 | Joback Method |
| cpg | 783.24 | J/mol×K | 959.54 | Joback Method |
| cpg | 792.13 | J/mol×K | 993.70 | Joback Method |
| cpg | 800.03 | J/mol×K | 1027.86 | Joback Method |
| cpg | 806.95 | J/mol×K | 1062.03 | 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=U376962&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |
| **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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