# Glutaric acid, 2-fluoro-6-(trifluoromethyl)benzyl heptyl ester

**Inchi:** InChI=1S/C20H26F4O4/c1-2-3-4-5-6-13-27-18(25)11-8-12-19(26)28-14-15-16(20(22,23)
**InchiKey:** HFAYFVLGICXNHP-UHFFFAOYSA-N
**Formula:** C20H26F4O4
**SMILES:** CCCCCCCOC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F
**Mol. weight [g/mol]:** 406.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1033.57 | kJ/mol | Joback Method |
| hf | -1525.33 | kJ/mol | Joback Method |
| hfus | 51.30 | kJ/mol | Joback Method |
| hvap | 77.46 | kJ/mol | Joback Method |
| log10ws | -6.53 | | Crippen Method |
| logp | 5.572 | | Crippen Method |
| mcvol | 290.860 | ml/mol | McGowan Method |
| pc | 1184.16 | kPa | Joback Method |
| rinpol | 2527.00 | | NIST Webbook |
| tb | 840.07 | K | Joback Method |
| tc | 1031.79 | K | Joback Method |
| tf | 515.72 | K | Joback Method |
| vc | 1.157 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 907.57 | J/mol×K | 840.07 | Joback Method |
| cpg | 922.28 | J/mol×K | 872.02 | Joback Method |
| cpg | 935.97 | J/mol×K | 903.98 | Joback Method |
| cpg | 948.67 | J/mol×K | 935.93 | Joback Method |
| cpg | 960.43 | J/mol×K | 967.89 | Joback Method |
| cpg | 971.28 | J/mol×K | 999.84 | Joback Method |
| cpg | 981.24 | J/mol×K | 1031.79 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377503&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |