# Glutaric acid, hexyl 4-(trifluoromethyl)benzyl ester

**Inchi:** InChI=1S/C19H25F3O4/c1-2-3-4-5-13-25-17(23)7-6-8-18(24)26-14-15-9-11-16(12-10-15
**InchiKey:** FUAIBNXKONSRSH-UHFFFAOYSA-N
**Formula:** C19H25F3O4
**SMILES:** CCCCCCOC(=O)CCCC(=O)OCc1ccc(C(F)(F)F)cc1
**Mol. weight [g/mol]:** 374.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -837.55 | kJ/mol | Joback Method |
| hf | -1297.11 | kJ/mol | Joback Method |
| hfus | 46.02 | kJ/mol | Joback Method |
| hvap | 75.39 | kJ/mol | Joback Method |
| log10ws | -5.78 | | Crippen Method |
| logp | 5.042 | | Crippen Method |
| mcvol | 275.000 | ml/mol | McGowan Method |
| pc | 1322.31 | kPa | Joback Method |
| rinpol | 2420.00 | | NIST Webbook |
| rinpol | 2420.00 | | NIST Webbook |
| tb | 812.94 | K | Joback Method |
| tc | 1004.64 | K | Joback Method |
| tf | 491.34 | K | Joback Method |
| vc | 1.083 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 842.80 | J/mol×K | 812.94 | Joback Method |
| cpg | 857.56 | J/mol×K | 844.89 | Joback Method |
| cpg | 871.33 | J/mol×K | 876.84 | Joback Method |
| cpg | 884.14 | J/mol×K | 908.79 | Joback Method |
| cpg | 896.01 | J/mol×K | 940.74 | Joback Method |
| cpg | 907.00 | J/mol×K | 972.69 | Joback Method |
| cpg | 917.13 | J/mol×K | 1004.64 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377582&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |