# Glutaric acid, hexyl 1-phenyl-2,2,2-trifluoroethyl ester

**Inchi:** InChI=1S/C19H25F3O4/c1-2-3-4-8-14-25-16(23)12-9-13-17(24)26-18(19(20,21)22)15-10

**InchiKey:** WNANFOOTMKQXMW-UHFFFAOYSA-N

**Formula:** C19H25F3O4

**SMILES:** CCCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F

**Mol. weight [g/mol]:** 374.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -830.36 | kJ/mol | Joback Method |
| hf | -1290.92 | kJ/mol | Joback Method |
| hfus | 42.88 | kJ/mol | Joback Method |
| hvap | 74.34 | kJ/mol | Joback Method |
| log10ws | -5.73 | | Crippen Method |
| logp | 5.127 | | Crippen Method |
| mcvol | 275.000 | ml/mol | McGowan Method |
| pc | 1344.71 | kPa | Joback Method |
| rinpol | 2179.00 | | NIST Webbook |
| tb | 807.52 | K | Joback Method |
| tc | 999.89 | K | Joback Method |
| tf | 463.82 | K | Joback Method |
| vc | 1.077 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 844.07 | J/mol×K | 807.52 | Joback Method |
| cpg | 859.03 | J/mol×K | 839.58 | Joback Method |
| cpg | 872.97 | J/mol×K | 871.64 | Joback Method |
| cpg | 885.93 | J/mol×K | 903.70 | Joback Method |
| cpg | 897.93 | J/mol×K | 935.77 | Joback Method |
| cpg | 909.03 | J/mol×K | 967.83 | Joback Method |
| cpg | 919.25 | J/mol×K | 999.89 | 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=U377368&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 |