# Glutaric acid, 1-(cyclohex-2-enyl)hex-3-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C22H30F8O4/c1-2-7-16(13-12-15-8-4-3-5-9-15)34-18(32)11-6-10-17(31)33-14

**InchiKey:** TZJGDXCTZGFXHQ-UHFFFAOYSA-N

**Formula:** C22H30F8O4

**SMILES:** CCCC(CCC1C=CCCC1)OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 510.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1833.91 | kJ/mol | Joback Method |
| hf | -2480.60 | kJ/mol | Joback Method |
| hfus | 46.72 | kJ/mol | Joback Method |
| hvap | 72.40 | kJ/mol | Joback Method |
| log10ws | -7.63 | | Crippen Method |
| logp | 6.719 | | Crippen Method |
| mcvol | 334.720 | ml/mol | McGowan Method |
| pc | 927.24 | kPa | Joback Method |
| rinpol | 2227.00 | | NIST Webbook |
| rinpol | 2227.00 | | NIST Webbook |
| tb | 857.64 | K | Joback Method |
| tc | 1050.06 | K | Joback Method |
| tf | 472.14 | K | Joback Method |
| vc | 1.333 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1120.90 | J/mol×K | 857.64 | Joback Method |
| cpg | 1137.32 | J/mol×K | 889.71 | Joback Method |
| cpg | 1152.54 | J/mol×K | 921.78 | Joback Method |
| cpg | 1166.66 | J/mol×K | 953.85 | Joback Method |
| cpg | 1179.75 | J/mol×K | 985.92 | Joback Method |
| cpg | 1191.88 | J/mol×K | 1017.99 | Joback Method |
| cpg | 1203.14 | J/mol×K | 1050.06 | Joback Method |

# Sources

| | |
|---|---|
| **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=U405515&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 |