# Glutaric acid, isohexyl 5-methoxy-3-methylpent-2-yl ester

**Inchi:** InChI=1S/C18H34O5/c1-14(2)8-7-12-22-17(19)9-6-10-18(20)23-16(4)15(3)11-13-21-5/h1

**InchiKey:** RYPHGUVDBIWEMM-UHFFFAOYSA-N

**Formula:** C18H34O5

**SMILES:** COCCC(C)C(C)OC(=O)CCCC(=O)OCCCC(C)C

**Mol. weight [g/mol]:** 330.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -479.48 | kJ/mol | Joback Method |
| hf | -1052.51 | kJ/mol | Joback Method |
| hfus | 38.57 | kJ/mol | Joback Method |
| hvap | 75.22 | kJ/mol | Joback Method |
| log10ws | -3.80 | | Crippen Method |
| logp | 3.740 | | Crippen Method |
| mcvol | 285.230 | ml/mol | McGowan Method |
| pc | 1233.74 | kPa | Joback Method |
| rinpol | 2162.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |
| tb | 784.92 | K | Joback Method |
| tc | 969.58 | K | Joback Method |
| tf | 414.17 | K | Joback Method |
| vc | 1.091 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 881.95 | J/mol×K | 784.92 | Joback Method |
| cpg | 899.52 | J/mol×K | 815.70 | Joback Method |
| cpg | 916.05 | J/mol×K | 846.47 | Joback Method |
| cpg | 931.55 | J/mol×K | 877.25 | Joback Method |
| cpg | 946.01 | J/mol×K | 908.03 | Joback Method |
| cpg | 959.45 | J/mol×K | 938.80 | Joback Method |
| cpg | 971.86 | J/mol×K | 969.58 | Joback Method |
| dvisc | 0.0012351 | Pa×s | 414.17 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0004857 | Pa×s | 475.96 | Joback Method |
| dvisc | 0.0002367 | Pa×s | 537.75 | Joback Method |
| dvisc | 0.0001338 | Pa×s | 599.55 | Joback Method |
| dvisc | 0.0000841 | Pa×s | 661.34 | Joback Method |
| dvisc | 0.0000573 | Pa×s | 723.13 | Joback Method |
| dvisc | 0.0000414 | Pa×s | 784.92 | 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=U358435&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |