# Glutaric acid, isohexyl 3-(2-methoxyethyl)heptyl ester

**Inchi:** InChI=1S/C21H40O5/c1-5-6-10-19(13-16-24-4)14-17-26-21(23)12-7-11-20(22)25-15-8-9

**InchiKey:** QQGQTVOYRSPIDO-UHFFFAOYSA-N

**Formula:** C21H40O5

**SMILES:** CCCCC(CCOC)CCOC(=O)CCCC(=O)OCCCC(C)C

**Mol. weight [g/mol]:** 372.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -451.78 | kJ/mol | Joback Method |
| hf | -1109.15 | kJ/mol | Joback Method |
| hfus | 49.86 | kJ/mol | Joback Method |
| hvap | 82.29 | kJ/mol | Joback Method |
| log10ws | -4.94 | | Crippen Method |
| logp | 4.912 | | Crippen Method |
| mcvol | 327.500 | ml/mol | McGowan Method |
| pc | 1012.30 | kPa | Joback Method |
| rinpol | 2485.00 | | NIST Webbook |
| tb | 854.00 | K | Joback Method |
| tc | 1046.11 | K | Joback Method |
| tf | 462.98 | K | Joback Method |
| vc | 1.266 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1063.08 | J/mol×K | 854.00 | Joback Method |
| cpg | 1143.18 | J/mol×K | 1014.09 | Joback Method |
| cpg | 1129.61 | J/mol×K | 982.07 | Joback Method |
| cpg | 1114.82 | J/mol×K | 950.06 | Joback Method |
| cpg | 1098.82 | J/mol×K | 918.04 | Joback Method |
| cpg | 1081.57 | J/mol×K | 886.02 | Joback Method |
| cpg | 1155.54 | J/mol×K | 1046.11 | Joback Method |
| dvisc | 0.0000288 | Pa×s | 854.00 | Joback Method |
| dvisc | 0.0000393 | Pa×s | 788.83 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000568 | Pa×s | 723.66 | Joback Method |
| dvisc | 0.0000882 | Pa×s | 658.49 | Joback Method |
| dvisc | 0.0001510 | Pa×s | 593.32 | Joback Method |
| dvisc | 0.0002952 | Pa×s | 528.15 | Joback Method |
| dvisc | 0.0006967 | Pa×s | 462.98 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358524&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 |

# 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 |

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