# Sebacic acid, 2-ethoxyethyl octyl ester

**Inchi:** InChI=1S/C22H42O5/c1-3-5-6-7-12-15-18-26-21(23)16-13-10-8-9-11-14-17-22(24)27-20
**InchiKey:** HWYFPZPKWILTKQ-UHFFFAOYSA-N
**Formula:** C22H42O5
**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOCC
**Mol. weight [g/mol]:** 386.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -438.48 | kJ/mol | Joback Method |
| hf | -1119.23 | kJ/mol | Joback Method |
| hfus | 59.50 | kJ/mol | Joback Method |
| hvap | 85.29 | kJ/mol | Joback Method |
| log10ws | -5.84 | | Crippen Method |
| logp | 5.591 | | Crippen Method |
| mcvol | 341.590 | ml/mol | McGowan Method |
| pc | 943.84 | kPa | Joback Method |
| rinpol | 2657.00 | | NIST Webbook |
| tb | 877.76 | K | Joback Method |
| tc | 1074.82 | K | Joback Method |
| tf | 504.25 | K | Joback Method |
| vc | 1.333 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1124.11 | J/mol×K | 877.76 | Joback Method |
| cpg | 1143.04 | J/mol×K | 910.60 | Joback Method |
| cpg | 1160.64 | J/mol×K | 943.45 | Joback Method |
| cpg | 1176.92 | J/mol×K | 976.29 | Joback Method |
| cpg | 1191.91 | J/mol×K | 1009.14 | Joback Method |
| cpg | 1205.60 | J/mol×K | 1041.98 | Joback Method |
| cpg | 1218.02 | J/mol×K | 1074.82 | Joback Method |
| dvisc | 0.0004546 | Pa×s | 504.25 | Joback Method |
| dvisc | 0.0002244 | Pa×s | 566.50 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001273 | Pa×s | 628.75 | Joback Method |
| dvisc | 0.0000800 | Pa×s | 691.00 | Joback Method |
| dvisc | 0.0000543 | Pa×s | 753.26 | Joback Method |
| dvisc | 0.0000391 | Pa×s | 815.51 | Joback Method |
| dvisc | 0.0000295 | Pa×s | 877.76 | Joback Method |

# Sources

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|---|---|
| **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=U355634&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |