# Sebacic acid, hexadecyl propyl ester

**Inchi:** InChI=1S/C29H56O4/c1-3-5-6-7-8-9-10-11-12-13-14-17-20-23-27-33-29(31)25-22-19-16
**InchiKey:** UQQYLKGYEFPEQI-UHFFFAOYSA-N
**Formula:** C29H56O4
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCC
**Mol. weight [g/mol]:** 468.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -274.54 | kJ/mol | Joback Method |
| hf | -1131.49 | kJ/mol | Joback Method |
| hfus | 76.44 | kJ/mol | Joback Method |
| hvap | 98.46 | kJ/mol | Joback Method |
| log10ws | -9.69 | | Crippen Method |
| logp | 9.085 | | Crippen Method |
| mcvol | 434.350 | ml/mol | McGowan Method |
| pc | 654.10 | kPa | Joback Method |
| rinpol | 3346.00 | | NIST Webbook |
| tb | 1015.50 | K | Joback Method |
| tc | 1268.62 | K | Joback Method |
| tf | 560.91 | K | Joback Method |
| vc | 1.708 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1539.74 | J/mol×K | 1015.50 | Joback Method |
| cpg | 1563.27 | J/mol×K | 1057.69 | Joback Method |
| cpg | 1584.52 | J/mol×K | 1099.87 | Joback Method |
| cpg | 1603.59 | J/mol×K | 1142.06 | Joback Method |
| cpg | 1620.57 | J/mol×K | 1184.25 | Joback Method |
| cpg | 1635.54 | J/mol×K | 1226.44 | Joback Method |
| cpg | 1648.61 | J/mol×K | 1268.62 | Joback Method |
| dvisc | 0.0002741 | Pa×s | 560.91 | Joback Method |
| dvisc | 0.0001230 | Pa×s | 636.67 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000654 | Pa×s | 712.44 | Joback Method |
| dvisc | 0.0000393 | Pa×s | 788.20 | Joback Method |
| dvisc | 0.0000258 | Pa×s | 863.97 | Joback Method |
| dvisc | 0.0000181 | Pa×s | 939.73 | Joback Method |
| dvisc | 0.0000134 | Pa×s | 1015.50 | Joback Method |

# Sources

**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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U354481&Units=SI

# 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