

# Sebacic acid, 2-ethylhexyl tridecyl ester

**Inchi:** InChI=1S/C31H60O4/c1-4-7-9-10-11-12-13-14-17-20-23-27-34-30(32)25-21-18-15-16-19  
**InchiKey:** PTZCBSXIEDCMQJ-UHFFFAOYSA-N  
**Formula:** C31H60O4  
**SMILES:** CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(CC)CCCC  
**Mol. weight [g/mol]:** 496.81

## Physical Properties

Property code	Value	Unit	Source
gf	-260.14	kJ/mol	Joback Method
hf	-1178.05	kJ/mol	Joback Method
hfus	78.10	kJ/mol	Joback Method
hvap	102.52	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	9.721		Crippen Method
mvol	462.530	ml/mol	McGowan Method
pc	596.63	kPa	Joback Method
rinpol	3460.00		NIST Webbook
rinpol	3460.00		NIST Webbook
tb	1060.82	K	Joback Method
tc	1339.85	K	Joback Method
tf	568.45	K	Joback Method
vc	1.813	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.04	J/molxK	1060.82	Joback Method
cpg	1695.80	J/molxK	1107.32	Joback Method
cpg	1717.77	J/molxK	1153.83	Joback Method
cpg	1737.10	J/molxK	1200.33	Joback Method
cpg	1753.92	J/molxK	1246.84	Joback Method
cpg	1768.37	J/molxK	1293.34	Joback Method
cpg	1780.59	J/molxK	1339.85	Joback Method
dvisc	0.0002323	Paxs	568.45	Joback Method

dvisc	0.0000955	Paxs	650.51	Joback Method
dvisc	0.0000479	Paxs	732.57	Joback Method
dvisc	0.0000276	Paxs	814.64	Joback Method
dvisc	0.0000176	Paxs	896.70	Joback Method
dvisc	0.0000121	Paxs	978.76	Joback Method
dvisc	0.0000088	Paxs	1060.82	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354209&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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