

Sebacic acid, oct-3-yl pentadecyl ester

Inchi:	InChI=1S/C33H64O4/c1-4-7-9-10-11-12-13-14-15-16-19-22-26-30-36-32(34)28-24-20-17
InchiKey:	NLCOSCYCHUMFF-UHFFFAOYSA-N
Formula:	C33H64O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCCC
Mol. weight [g/mol]:	524.86

Physical Properties

Property code	Value	Unit	Source
gf	-243.30	kJ/mol	Joback Method
hf	-1219.33	kJ/mol	Joback Method
hfus	83.28	kJ/mol	Joback Method
hvap	106.98	kJ/mol	Joback Method
log10ws	-11.47		Crippen Method
logp	10.644		Crippen Method
mvol	490.710	ml/mol	McGowan Method
pc	544.37	kPa	Joback Method
rinpol	3262.00		NIST Webbook
rinpol	3262.00		NIST Webbook
tb	1106.58	K	Joback Method
tc	1421.70	K	Joback Method
tf	590.99	K	Joback Method
vc	1.925	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.88	J/molxK	1106.58	Joback Method
cpg	1829.39	J/molxK	1159.10	Joback Method
cpg	1852.41	J/molxK	1211.62	Joback Method
cpg	1872.15	J/molxK	1264.14	Joback Method
cpg	1888.82	J/molxK	1316.66	Joback Method
cpg	1902.66	J/molxK	1369.18	Joback Method
cpg	1913.88	J/molxK	1421.70	Joback Method
dvisc	0.0001733	Paxs	590.99	Joback Method

dvisc	0.0000704	Paxs	676.92	Joback Method
dvisc	0.0000351	Paxs	762.85	Joback Method
dvisc	0.0000201	Paxs	848.78	Joback Method
dvisc	0.0000128	Paxs	934.72	Joback Method
dvisc	0.0000087	Paxs	1020.65	Joback Method
dvisc	0.0000064	Paxs	1106.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U416839&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

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