

Sebacic acid, 6-ethyloct-3-yl undecyl ester

Inchi: InChI=1S/C31H60O4/c1-5-9-10-11-12-13-16-19-22-27-34-30(32)23-20-17-14-15-18-21-2
InchiKey: WKNSMOYZGPIHEU-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCC(CC)CC
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-262.58	kJ/mol	Joback Method
hf	-1183.33	kJ/mol	Joback Method
hfus	74.57	kJ/mol	Joback Method
hvap	102.14	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.719		Crippen Method
mvol	462.530	ml/mol	McGowan Method
pc	598.97	kPa	Joback Method
rinpol	3361.00		NIST Webbook
rinpol	3361.00		NIST Webbook
tb	1060.38	K	Joback Method
tc	1335.48	K	Joback Method
tf	553.45	K	Joback Method
vc	1.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.19	J/molxK	1060.38	Joback Method
cpg	1695.52	J/molxK	1106.23	Joback Method
cpg	1717.12	J/molxK	1152.08	Joback Method
cpg	1736.12	J/molxK	1197.93	Joback Method
cpg	1752.66	J/molxK	1243.78	Joback Method
cpg	1766.86	J/molxK	1289.63	Joback Method
cpg	1778.86	J/molxK	1335.48	Joback Method
dvisc	0.0002633	Paxs	553.45	Joback Method

dvisc	0.0001001	Paxs	637.94	Joback Method
dvisc	0.0000477	Paxs	722.43	Joback Method
dvisc	0.0000266	Paxs	806.91	Joback Method
dvisc	0.0000165	Paxs	891.40	Joback Method
dvisc	0.0000112	Paxs	975.89	Joback Method
dvisc	0.0000080	Paxs	1060.38	Joback Method

Sources

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=U354192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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