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

Inchi: InChI=1S/C33H64O4/c1-5-9-10-11-12-13-14-15-18-21-24-29-36-32(34)25-22-19-16-17-2

InchiKey: YSFOTZQCVDROIA-UHFFFAOYSA-N

Formula: C33H64O4

SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCC(CC)CC

Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-245.74	kJ/mol	Joback Method
hf	-1224.61	kJ/mol	Joback Method
hfus	79.75	kJ/mol	Joback Method
hvap	106.59	kJ/mol	Joback Method
log10ws	-11.23		Crippen Method
logp	10.500		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	546.41	kPa	Joback Method
rinpol	3576.00		NIST Webbook
rinpol	3576.00		NIST Webbook
tb	1106.14	K	Joback Method
tc	1416.02	K	Joback Method
tf	575.99	K	Joback Method
vc	1.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.92	J/mol×K	1106.14	Joback Method
cpg	1828.88	J/mol×K	1157.79	Joback Method
cpg	1851.43	J/mol×K	1209.43	Joback Method
cpg	1870.77	J/mol×K	1261.08	Joback Method
cpg	1887.12	J/mol×K	1312.73	Joback Method
cpg	1900.68	J/mol×K	1364.37	Joback Method
cpg	1911.65	J/mol×K	1416.02	Joback Method
dvisc	0.0001947	Pa×s	575.99	Joback Method

dvisc	0.0000733	Pa×s	664.35	Joback Method
dvisc	0.0000347	Pa×s	752.71	Joback Method
dvisc	0.0000192	Pa×s	841.06	Joback Method
dvisc	0.0000119	Pa×s	929.42	Joback Method
dvisc	0.0000080	Pa×s	1017.78	Joback Method
dvisc	0.0000058	Pa×s	1106.14	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=U354194&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