Sebacic acid, pentadecyl 2-propylpentyl ester

Inchi: InChI=1S/C33H64O4/c1-4-7-8-9-10-11-12-13-14-15-18-21-24-29-36-32(34)27-22-19-16-
InchiKey: CATRYSQLGZOZLQ-UHFFFAOYSA-N
Formula: C33H64O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(CCC)CCC
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	-11.12		Crippen Method
logp	10.501		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	544.37	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	1106.58	K	Joback Method
tc	1421.70	K	Joback Method
tf	590.99	K	Joback Method
vc	1.925	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000704	Pa×s	676.92	Joback Method
dvisc	0.0000351	Pa×s	762.85	Joback Method
dvisc	0.0000201	Pa×s	848.78	Joback Method
dvisc	0.0000128	Pa×s	934.72	Joback Method
dvisc	0.0000087	Pa×s	1020.65	Joback Method
dvisc	0.0000064	Pa×s	1106.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416220&Units=SI
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

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