Sebacic acid, 3,3-dimethylbut-2-yl pentadecyl ester

Inchi: InChI=1S/C31H60O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-34-29(32)25-22-19-16-

InchiKey: SBSBABVRHXVGHB-UHFFFAOYSA-N

Formula: C31H60O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-257.30	kJ/mol	Joback Method
hf	-1186.80	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	101.23	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.719		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	602.21	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1057.59	K	Joback Method
tc	1325.01	K	Joback Method
tf	570.87	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.72	J/mol×K	1057.59	Joback Method
cpg	1770.52	J/mol×K	1280.44	Joback Method
cpg	1754.54	J/mol×K	1235.87	Joback Method
cpg	1736.73	J/mol×K	1191.30	Joback Method
cpg	1716.93	J/mol×K	1146.73	Joback Method
cpg	1694.98	J/mol×K	1102.16	Joback Method
cpg	1784.83	J/mol×K	1325.01	Joback Method
dvisc	0.0000066	Pa×s	1057.59	Joback Method

dvisc	0.0000092	Pa×s	976.47	Joback Method
dvisc	0.0000136	Pa×s	895.35	Joback Method
dvisc	0.0000218	Pa×s	814.23	Joback Method
dvisc	0.0000389	Pa×s	733.11	Joback Method
dvisc	0.0000799	Pa×s	651.99	Joback Method
dvisc	0.0002015	Pa×s	570.87	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=U355609&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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