Sebacic acid, 2,4-dimethylpent-3-yl tetradecyl ester

Inchi: InChI=1S/C31H60O4/c1-6-7-8-9-10-11-12-13-14-17-20-23-26-34-29(32)24-21-18-15-16-

InchiKey: KQRQQLMMHHHLBA-UHFFFAOYSA-N

Formula: C31H60O4

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

Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-265.02	kJ/mol	Joback Method
hf	-1188.61	kJ/mol	Joback Method
hfus	71.05	kJ/mol	Joback Method
hvap	101.75	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.575		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	601.32	kPa	Joback Method
rinpol	3328.00		NIST Webbook
rinpol	3328.00		NIST Webbook
tb	1059.94	K	Joback Method
tc	1331.32	K	Joback Method
tf	538.45	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.35	J/mol×K	1059.94	Joback Method
cpg	1765.42	J/mol×K	1286.09	Joback Method
cpg	1751.46	J/mol×K	1240.86	Joback Method
cpg	1735.20	J/mol×K	1195.63	Joback Method
cpg	1716.51	J/mol×K	1150.40	Joback Method
cpg	1695.27	J/mol×K	1105.17	Joback Method
cpg	1777.20	J/mol×K	1331.32	Joback Method
dvisc	0.0000073	Pa×s	1059.94	Joback Method

dvisc	0.0000103	Pa×s	973.03	Joback Method
dvisc	0.0000155	Pa×s	886.11	Joback Method
dvisc	0.0000256	Pa×s	799.20	Joback Method
dvisc	0.0000477	Pa×s	712.28	Joback Method
dvisc	0.0001056	Pa×s	625.37	Joback Method
dvisc	0.0003028	Pa×s	538.45	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=U355436&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