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

Inchi: InChI=1S/C33H64O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-25-28-36-31(34)26-23-20-

InchiKey: QYJZTTFFEGTYDY-UHFFFAOYSA-N

Formula: C33H64O4

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

Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-248.18	kJ/mol	Joback Method
hf	-1229.89	kJ/mol	Joback Method
hfus	76.23	kJ/mol	Joback Method
hvap	106.20	kJ/mol	Joback Method
log10ws	-10.99		Crippen Method
logp	10.356		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	548.46	kPa	Joback Method
rinpol	3566.00		NIST Webbook
tb	1105.70	K	Joback Method
tc	1410.58	K	Joback Method
tf	560.99	K	Joback Method
vc	1.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.96	J/mol×K	1105.70	Joback Method
cpg	1898.77	J/mol×K	1359.76	Joback Method
cpg	1885.48	J/mol×K	1308.95	Joback Method
cpg	1869.46	J/mol×K	1258.14	Joback Method
cpg	1850.50	J/mol×K	1207.33	Joback Method
cpg	1828.39	J/mol×K	1156.51	Joback Method
cpg	1909.51	J/mol×K	1410.58	Joback Method
dvisc	0.0000052	Pa×s	1105.70	Joback Method
dvisc	0.0000074	Pa×s	1014.92	Joback Method

dvisc	0.0000112	Pa×s	924.13	Joback Method
dvisc	0.0000184	Pa×s	833.35	Joback Method
dvisc	0.0000345	Pa×s	742.56	Joback Method
dvisc	0.0000768	Pa×s	651.77	Joback Method
dvisc	0.0002217	Pa×s	560.99	Joback Method

Sources

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=U355438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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