Sebacic acid, neopentyl tetradecyl ester

Inchi: InChI=1S/C29H56O4/c1-5-6-7-8-9-10-11-12-13-16-19-22-25-32-27(30)23-20-17-14-15-1
InchiKey: BDBWUFOKRMZRLQ-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-1140.24	kJ/mol	Joback Method
hfus	69.03	kJ/mol	Joback Method
hvap	97.16	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	660.51	kPa	Joback Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook
tb	1012.27	K	Joback Method
tc	1256.59	K	Joback Method
tf	563.33	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.29	J/mol×K	1012.27	Joback Method
cpg	1562.26	J/mol×K	1052.99	Joback Method
cpg	1583.28	J/mol×K	1093.71	Joback Method
cpg	1602.46	J/mol×K	1134.43	Joback Method
cpg	1619.92	J/mol×K	1175.15	Joback Method
cpg	1635.76	J/mol×K	1215.87	Joback Method
cpg	1650.11	J/mol×K	1256.59	Joback Method
dvisc	0.0002393	Pa×s	563.33	Joback Method

dvisc	0.0001037	Pa×s	638.15	Joback Method
dvisc	0.0000535	Pa×s	712.98	Joback Method
dvisc	0.0000313	Pa×s	787.80	Joback Method
dvisc	0.0000201	Pa×s	862.62	Joback Method
dvisc	0.0000139	Pa×s	937.45	Joback Method
dvisc	0.0000101	Pa×s	1012.27	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=U354475&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