

Sebacic acid, neopentyl tridecyl ester

Inchi:	InChI=1S/C28H54O4/c1-5-6-7-8-9-10-11-12-15-18-21-24-31-26(29)22-19-16-13-14-17-2
InchiKey:	HBSLUFBRKCUIX-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-1119.60	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	94.94	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.551		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinsol	3130.00		NIST Webbook
tb	989.39	K	Joback Method
tc	1222.65	K	Joback Method
tf	552.06	K	Joback Method
vc	1.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.13	J/molxK	989.39	Joback Method
cpg	1496.36	J/molxK	1028.27	Joback Method
cpg	1516.80	J/molxK	1067.14	Joback Method
cpg	1535.55	J/molxK	1106.02	Joback Method
cpg	1552.70	J/molxK	1144.89	Joback Method
cpg	1568.34	J/molxK	1183.77	Joback Method
cpg	1582.58	J/molxK	1222.65	Joback Method
dvisc	0.0002762	Paxs	552.06	Joback Method
dvisc	0.0001206	Paxs	624.95	Joback Method

dvisc	0.0000626	Paxs	697.84	Joback Method
dvisc	0.0000368	Paxs	770.72	Joback Method
dvisc	0.0000237	Paxs	843.61	Joback Method
dvisc	0.0000164	Paxs	916.50	Joback Method
dvisc	0.0000119	Paxs	989.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U354474&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

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