

Sebacic acid, 2-chloropropyl propyl ester

Inchi:	InChI=1S/C16H29ClO4/c1-3-12-20-15(18)10-8-6-4-5-7-9-11-16(19)21-13-14(2)17/h14H,1
InchiKey:	ZKJVJVWGGALPMD-UHFFFAOYSA-N
Formula:	C16H29ClO4
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	320.85

Physical Properties

Property code	Value	Unit	Source
gf	-398.37	kJ/mol	Joback Method
hf	-884.19	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.231		Crippen Method
mcvol	263.420	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpola	2181.00		NIST Webbook
tb	755.05	K	Joback Method
tc	938.27	K	Joback Method
tf	429.32	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.33	J/molxK	755.05	Joback Method
cpg	781.21	J/molxK	785.59	Joback Method
cpg	796.21	J/molxK	816.12	Joback Method
cpg	810.35	J/molxK	846.66	Joback Method
cpg	823.63	J/molxK	877.19	Joback Method
cpg	836.07	J/molxK	907.73	Joback Method
cpg	847.68	J/molxK	938.27	Joback Method
dvisc	0.0012042	Paxs	429.32	Joback Method
dvisc	0.0005848	Paxs	483.61	Joback Method

dvisc	0.0003285	Paxs	537.90	Joback Method
dvisc	0.0002052	Paxs	592.18	Joback Method
dvisc	0.0001387	Paxs	646.47	Joback Method
dvisc	0.0000996	Paxs	700.76	Joback Method
dvisc	0.0000750	Paxs	755.05	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=U355442&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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