Sebacic acid, di(2-chloropropyl) ester

Inchi: InChI=1S/C16H28Cl2O4/c1-13(17)11-21-15(19)9-7-5-3-4-6-8-10-16(20)22-12-14(2)18/h1
InchiKey: RQXYNAROVWNORZ-UHFFFAOYSA-N
Formula: C16H28Cl2O4
SMILES: CC(Cl)COC(=O)CCCCCCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 355.30

Physical Properties

Property code	Value	Unit	Source
gf	-412.74	kJ/mol	Joback Method
hf	-905.21	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.448		Crippen Method
mcvol	275.660	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	792.04	K	Joback Method
tc	982.16	K	Joback Method
tf	444.24	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.14	J/mol×K	792.04	Joback Method
cpg	861.34	J/mol×K	950.48	Joback Method
cpg	849.92	J/mol×K	918.79	Joback Method
cpg	837.60	J/mol×K	887.10	Joback Method
cpg	824.37	J/mol×K	855.41	Joback Method
cpg	810.22	J/mol×K	823.73	Joback Method
cpg	871.89	J/mol×K	982.16	Joback Method
dvisc	0.0000594	Pa×s	792.04	Joback Method

dvisc	0.0000799	Pa×s	734.07	Joback Method
dvisc	0.0001131	Pa×s	676.11	Joback Method
dvisc	0.0001707	Pa×s	618.14	Joback Method
dvisc	0.0002808	Pa×s	560.17	Joback Method
dvisc	0.0005180	Pa×s	502.21	Joback Method
dvisc	0.0011212	Pa×s	444.24	Joback Method

Sources

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=U355448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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