Succinic acid, 8-chlorooctyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H23Cl3O4/c15-9-5-3-1-2-4-6-10-20-13(18)7-8-14(19)21-11-12(16)17/h12H

InchiKey: RJJDUTIEVZWFOK-UHFFFAOYSA-N

Formula: C14H23Cl3O4

SMILES: O=C(CCC(=O)OCC(Cl)Cl)OCCCCCCCCCl

Mol. weight [g/mol]: 361.69

Physical Properties

Property code	Value	Unit	Source
gf	-439.07	kJ/mol	Joback Method
hf	-874.39	kJ/mol	Joback Method
hfus	46.66	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.236		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	784.15	K	Joback Method
tc	976.41	K	Joback Method
tf	466.62	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.74	J/mol×K	784.15	Joback Method
cpg	766.63	J/mol×K	944.37	Joback Method
cpg	756.70	J/mol×K	912.32	Joback Method
cpg	745.95	J/mol×K	880.28	Joback Method
cpg	734.38	J/mol×K	848.24	Joback Method
cpg	721.98	J/mol×K	816.19	Joback Method
cpg	775.77	J/mol×K	976.41	Joback Method
dvisc	0.0000743	Pa×s	784.15	Joback Method

dvisc	0.0000973	Pa×s	731.23	Joback Method
dvisc	0.0001328	Pa×s	678.31	Joback Method
dvisc	0.0001911	Pa×s	625.38	Joback Method
dvisc	0.0002941	Pa×s	572.46	Joback Method
dvisc	0.0004942	Pa×s	519.54	Joback Method
dvisc	0.0009342	Pa×s	466.62	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=U390526&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