Succinic acid, 2,2-dichloroethyl hexyl ester

Inchi: InChI=1S/C12H20Cl2O4/c1-2-3-4-5-8-17-11(15)6-7-12(16)18-9-10(13)14/h10H,2-9H2,1H
InchiKey: LIMINAVCMQPAHE-UHFFFAOYSA-N
Formula: C12H20Cl2O4
SMILES: CCCCCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-443.98	kJ/mol	Joback Method
hf	-817.37	kJ/mol	Joback Method
hfus	37.28	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.237		Crippen Method
mcvol	219.300	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	700.96	K	Joback Method
tc	889.73	K	Joback Method
tf	414.16	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.54	J/mol×K	700.96	Joback Method
cpg	586.79	J/mol×K	732.42	Joback Method
cpg	599.31	J/mol×K	763.88	Joback Method
cpg	611.11	J/mol×K	795.34	Joback Method
cpg	622.19	J/mol×K	826.80	Joback Method
cpg	632.56	J/mol×K	858.26	Joback Method
cpg	642.22	J/mol×K	889.73	Joback Method
dvisc	0.0014300	Pa×s	414.16	Joback Method

dvisc	0.0007549	Pa×s	461.96	Joback Method
dvisc	0.0004492	Pa×s	509.76	Joback Method
dvisc	0.0002922	Pa×s	557.56	Joback Method
dvisc	0.0002034	Pa×s	605.36	Joback Method
dvisc	0.0001493	Pa×s	653.16	Joback Method
dvisc	0.0001143	Pa×s	700.96	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=U389536&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