Succinic acid, hept-2-yl 2,2-dichloroethyl ester

Inchi: InChI=1S/C13H22Cl2O4/c1-3-4-5-6-10(2)19-13(17)8-7-12(16)18-9-11(14)15/h10-11H,3-9

InchiKey: KAGSUOXBROXGDK-UHFFFAOYSA-N

Formula: C13H22Cl2O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 313.22

Physical Properties

Property code	Value	Unit	Source
gf	-438.00	kJ/mol	Joback Method
hf	-843.29	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.626		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook
tb	723.40	K	Joback Method
tc	913.79	K	Joback Method
tf	410.43	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.65	J/mol×K	723.40	Joback Method
cpg	641.58	J/mol×K	755.13	Joback Method
cpg	654.71	J/mol×K	786.86	Joback Method
cpg	667.05	J/mol×K	818.59	Joback Method
cpg	678.60	J/mol×K	850.32	Joback Method
cpg	689.37	J/mol×K	882.05	Joback Method
cpg	699.36	J/mol×K	913.79	Joback Method
dvisc	0.0015655	Pa×s	410.43	Joback Method

dvisc	0.0007478	Pa×s	462.59	Joback Method
dvisc	0.0004149	Pa×s	514.75	Joback Method
dvisc	0.0002565	Pa×s	566.91	Joback Method
dvisc	0.0001720	Pa×s	619.08	Joback Method
dvisc	0.0001227	Pa×s	671.24	Joback Method
dvisc	0.0000919	Pa×s	723.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390518&Units=SI
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

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