Succinic acid, 2,2-dichloroethyl 1-cyclopentylethyl ester

Inchi: InChI=1S/C13H20Cl2O4/c1-9(10-4-2-3-5-10)19-13(17)7-6-12(16)18-8-11(14)15/h9-11H,2
InchiKey: QNNJUBWLHQJVOQ-UHFFFAOYSA-N
Formula: C13H20Cl2O4
SMILES: CC(OC(=O)CCC(=O)OCC(Cl)Cl)C1CCCC1
Mol. weight [g/mol]: 311.20

Physical Properties

Property code	Value	Unit	Source
gf	-401.45	kJ/mol	Joback Method
hf	-782.81	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.235		Crippen Method
mcvol	222.530	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	738.68	K	Joback Method
tc	949.03	K	Joback Method
tf	421.33	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.65	J/mol×K	738.68	Joback Method
cpg	683.02	J/mol×K	913.97	Joback Method
cpg	671.99	J/mol×K	878.91	Joback Method
cpg	659.96	J/mol×K	843.86	Joback Method
cpg	646.90	J/mol×K	808.80	Joback Method
cpg	632.81	J/mol×K	773.74	Joback Method
cpg	693.07	J/mol×K	949.03	Joback Method
dvisc	0.0001331	Pa×s	738.68	Joback Method

dvisc	0.0001746	Pa×s	685.79	Joback Method
dvisc	0.0002397	Pa×s	632.90	Joback Method
dvisc	0.0003487	Pa×s	580.00	Joback Method
dvisc	0.0005467	Pa×s	527.11	Joback Method
dvisc	0.0009478	Pa×s	474.22	Joback Method
dvisc	0.0018866	Pa×s	421.33	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=U391411&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