Succinic acid, 2,2-dichloroethyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C13H22Cl2O4/c1-8(2)13(9(3)4)19-12(17)6-5-11(16)18-7-10(14)15/h8-10,13H,5

InchiKey: KBONSUMDTSKWBM-UHFFFAOYSA-N

Formula: C13H22Cl2O4

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

Mol. weight [g/mol]: 313.22

Physical Properties

Property code	Value	Unit	Source
gf	-442.88	kJ/mol	Joback Method
hf	-853.85	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.337		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	722.52	K	Joback Method
tc	918.29	K	Joback Method
tf	380.43	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.73	J/mol×K	722.52	Joback Method
cpg	643.09	J/mol×K	755.15	Joback Method
cpg	656.58	J/mol×K	787.78	Joback Method
cpg	669.22	J/mol×K	820.41	Joback Method
cpg	681.01	J/mol×K	853.04	Joback Method
cpg	691.95	J/mol×K	885.66	Joback Method
cpg	702.06	J/mol×K	918.29	Joback Method
dvisc	0.0024492	Pa×s	380.43	Joback Method

dvisc	0.0009498	Pa×s	437.44	Joback Method
dvisc	0.0004582	Pa×s	494.46	Joback Method
dvisc	0.0002570	Pa×s	551.48	Joback Method
dvisc	0.0001607	Pa×s	608.49	Joback Method
dvisc	0.0001089	Pa×s	665.50	Joback Method
dvisc	0.0000784	Pa×s	722.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390504&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

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