Succinic acid, 2,2-dichloroethyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C11H18Cl2O4/c1-7(2)8(3)17-11(15)5-4-10(14)16-6-9(12)13/h7-9H,4-6H2,1-3H

InchiKey: APFQDRAVAMFWPT-UHFFFAOYSA-N

Formula: C11H18Cl2O4

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

Mol. weight [g/mol]: 285.16

Physical Properties

Property code	Value	Unit	Source
gf	-457.28	kJ/mol	Joback Method
hf	-807.29	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.701		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1693.00		NIST Webbook
tb	677.20	K	Joback Method
tc	873.45	K	Joback Method
tf	372.89	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.29	J/mol×K	677.20	Joback Method
cpg	535.47	J/mol×K	709.91	Joback Method
cpg	547.90	J/mol×K	742.62	Joback Method
cpg	559.60	J/mol×K	775.33	Joback Method
cpg	570.55	J/mol×K	808.04	Joback Method
cpg	580.77	J/mol×K	840.75	Joback Method
cpg	590.25	J/mol×K	873.45	Joback Method
dvisc	0.0023975	Pa×s	372.89	Joback Method

dvisc	0.0010610	Pa×s	423.61	Joback Method
dvisc	0.0005590	Pa×s	474.33	Joback Method
dvisc	0.0003333	Pa×s	525.05	Joback Method
dvisc	0.0002177	Pa×s	575.76	Joback Method
dvisc	0.0001523	Pa×s	626.48	Joback Method
dvisc	0.0001125	Pa×s	677.20	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=U390582&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