

Succinic acid, 2,2-dichloroethyl propyl ester

Inchi:	InChI=1S/C9H14Cl2O4/c1-2-5-14-8(12)3-4-9(13)15-6-7(10)11/h7H,2-6H2,1H3
InchiKey:	FJMPKWLUBAMQEB-UHFFFAOYSA-N
Formula:	C9H14Cl2O4
SMILES:	CCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	257.11

Physical Properties

Property code	Value	Unit	Source
gf	-469.24	kJ/mol	Joback Method
hf	-755.45	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.067		Crippen Method
mcvol	177.030	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinsol	1589.00		NIST Webbook
tb	632.32	K	Joback Method
tc	826.21	K	Joback Method
tf	380.35	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.84	J/molxK	632.32	Joback Method
cpg	432.25	J/molxK	664.64	Joback Method
cpg	443.08	J/molxK	696.95	Joback Method
cpg	453.33	J/molxK	729.27	Joback Method
cpg	462.98	J/molxK	761.58	Joback Method
cpg	472.05	J/molxK	793.90	Joback Method
cpg	480.52	J/molxK	826.21	Joback Method
dvisc	0.0018392	Paxs	380.35	Joback Method
dvisc	0.0010147	Paxs	422.34	Joback Method

dvisc	0.0006234	Paxs	464.34	Joback Method
dvisc	0.0004153	Paxs	506.33	Joback Method
dvisc	0.0002944	Paxs	548.33	Joback Method
dvisc	0.0002191	Paxs	590.32	Joback Method
dvisc	0.0001696	Paxs	632.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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