

Succinic acid, 2,2-dichloroethyl ethyl ester

Inchi:	InChI=1S/C8H12Cl2O4/c1-2-13-7(11)3-4-8(12)14-5-6(9)10/h6H,2-5H2,1H3
InchiKey:	PFNFXPLZQOXXMK-UHFFFAOYSA-N
Formula:	C8H12Cl2O4
SMILES:	CCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	243.08

Physical Properties

Property code	Value	Unit	Source
gf	-477.66	kJ/mol	Joback Method
hf	-734.81	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.677		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	609.44	K	Joback Method
tc	805.72	K	Joback Method
tf	369.08	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.93	J/molxK	609.44	Joback Method
cpg	383.56	J/molxK	642.15	Joback Method
cpg	393.66	J/molxK	674.87	Joback Method
cpg	403.23	J/molxK	707.58	Joback Method
cpg	412.26	J/molxK	740.30	Joback Method
cpg	420.74	J/molxK	773.01	Joback Method
cpg	428.67	J/molxK	805.72	Joback Method
dvisc	0.0019734	Paxs	369.08	Joback Method

dvisc	0.0011065	Paxs	409.14	Joback Method
dvisc	0.0006879	Paxs	449.20	Joback Method
dvisc	0.0004623	Paxs	489.26	Joback Method
dvisc	0.0003299	Paxs	529.32	Joback Method
dvisc	0.0002469	Paxs	569.38	Joback Method
dvisc	0.0001919	Paxs	609.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349402&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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