

Succinic acid, 2,2-dichloroethyl phenethyl ester

Inchi:	InChI=1S/C14H16Cl2O4/c15-12(16)10-20-14(18)7-6-13(17)19-9-8-11-4-2-1-3-5-11/h1-5,
InchiKey:	KXYPMCUBOIWQCN-UHFFFAOYSA-N
Formula:	C14H16Cl2O4
SMILES:	O=C(CCC(=O)OCC(Cl)Cl)OCCc1ccccc1
Mol. weight [g/mol]:	319.18

Physical Properties

Property code	Value	Unit	Source
gf	-314.73	kJ/mol	Joback Method
hf	-622.12	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.899		Crippen Method
mvol	223.720	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	773.40	K	Joback Method
tc	988.60	K	Joback Method
tf	463.12	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.21	J/molxK	773.40	Joback Method
cpg	604.72	J/molxK	809.27	Joback Method
cpg	616.24	J/molxK	845.13	Joback Method
cpg	626.80	J/molxK	881.00	Joback Method
cpg	636.42	J/molxK	916.86	Joback Method
cpg	645.11	J/molxK	952.73	Joback Method
cpg	652.90	J/molxK	988.60	Joback Method
dvisc	0.0009669	Paxs	463.12	Joback Method

dvisc	0.0005292	Paxs	514.83	Joback Method
dvisc	0.0003233	Paxs	566.55	Joback Method
dvisc	0.0002145	Paxs	618.26	Joback Method
dvisc	0.0001516	Paxs	669.97	Joback Method
dvisc	0.0001126	Paxs	721.69	Joback Method
dvisc	0.0000871	Paxs	773.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389745&Units=SI

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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