

Succinic acid, 2,2-dichloroethyl 2-pentyl ester

Inchi:	InChI=1S/C11H18Cl2O4/c1-3-4-8(2)17-11(15)6-5-10(14)16-7-9(12)13/h8-9H,3-7H2,1-2H
InchiKey:	XLBAEKFEKFTWFK-UHFFFAOYSA-N
Formula:	C11H18Cl2O4
SMILES:	CCCC(C)OC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	285.16

Physical Properties

Property code	Value	Unit	Source
gf	-454.84	kJ/mol	Joback Method
hf	-802.01	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.845		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinsol	1682.00		NIST Webbook
tb	677.64	K	Joback Method
tc	870.74	K	Joback Method
tf	387.89	K	Joback Method
vc	0.785	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.77	J/molxK	677.64	Joback Method
cpg	534.70	J/molxK	709.82	Joback Method
cpg	546.93	J/molxK	742.01	Joback Method
cpg	558.45	J/molxK	774.19	Joback Method
cpg	569.26	J/molxK	806.37	Joback Method
cpg	579.37	J/molxK	838.56	Joback Method
cpg	588.77	J/molxK	870.74	Joback Method
dvisc	0.0019110	Paxs	387.89	Joback Method
dvisc	0.0009359	Paxs	436.18	Joback Method

dvisc	0.0005285	Paxs	484.47	Joback Method
dvisc	0.0003310	Paxs	532.76	Joback Method
dvisc	0.0002241	Paxs	581.06	Joback Method
dvisc	0.0001610	Paxs	629.35	Joback Method
dvisc	0.0001213	Paxs	677.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370897&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

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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