

Succinic acid, 2,2-dichloroethyl neopentyl ester

Inchi:	InChI=1S/C11H18Cl2O4/c1-11(2,3)7-17-10(15)5-4-9(14)16-6-8(12)13/h8H,4-7H2,1-3H3
InchiKey:	KYTJDDFPQLHXAC-UHFFFAOYSA-N
Formula:	C11H18Cl2O4
SMILES:	CC(C)(C)COC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	285.16

Physical Properties

Property code	Value	Unit	Source
gf	-449.56	kJ/mol	Joback Method
hf	-805.48	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.703		Crippen Method
mvol	205.210	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	674.85	K	Joback Method
tc	873.79	K	Joback Method
tf	405.31	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.21	J/molxK	674.85	Joback Method
cpg	537.29	J/molxK	708.01	Joback Method
cpg	549.57	J/molxK	741.16	Joback Method
cpg	561.09	J/molxK	774.32	Joback Method
cpg	571.85	J/molxK	807.47	Joback Method
cpg	581.88	J/molxK	840.63	Joback Method
cpg	591.19	J/molxK	873.79	Joback Method
dvisc	0.0016011	Paxs	405.31	Joback Method

dvisc	0.0008229	Paxs	450.23	Joback Method
dvisc	0.0004772	Paxs	495.16	Joback Method
dvisc	0.0003030	Paxs	540.08	Joback Method
dvisc	0.0002063	Paxs	585.00	Joback Method
dvisc	0.0001484	Paxs	629.93	Joback Method
dvisc	0.0001115	Paxs	674.85	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=U389579&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

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