

Succinic acid, 2,2-dichloroethyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C8H9Cl5O4/c9-5(10)3-16-6(14)1-2-7(15)17-4-8(11,12)13/h5H,1-4H2
InchiKey:	DNAYOKRJOZXYBX-UHFFFAOYSA-N
Formula:	C8H9Cl5O4
SMILES:	O=C(CCC(=O)OCC(Cl)(Cl)Cl)OCC(Cl)Cl
Mol. weight [g/mol]:	346.42

Physical Properties

Property code	Value	Unit	Source
gf	-510.61	kJ/mol	Joback Method
hf	-790.78	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.027		Crippen Method
mvol	199.660	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	718.50	K	Joback Method
tc	935.97	K	Joback Method
tf	461.26	K	Joback Method
vc	0.759	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.93	J/molxK	718.50	Joback Method
cpg	450.39	J/molxK	754.74	Joback Method
cpg	458.16	J/molxK	790.99	Joback Method
cpg	465.25	J/molxK	827.23	Joback Method
cpg	471.70	J/molxK	863.48	Joback Method
cpg	477.50	J/molxK	899.72	Joback Method
cpg	482.70	J/molxK	935.97	Joback Method
dvisc	0.0010757	Paxs	461.26	Joback Method

dvisc	0.0006261	Paxs	504.13	Joback Method
dvisc	0.0003967	Paxs	547.01	Joback Method
dvisc	0.0002686	Paxs	589.88	Joback Method
dvisc	0.0001917	Paxs	632.75	Joback Method
dvisc	0.0001428	Paxs	675.63	Joback Method
dvisc	0.0001102	Paxs	718.50	Joback Method

Sources

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=U390233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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