

Succinic acid, 2,2-dichloroethyl heptyl ester

Inchi:	InChI=1S/C13H22Cl2O4/c1-2-3-4-5-6-9-18-12(16)7-8-13(17)19-10-11(14)15/h11H,2-10H
InchiKey:	XYHOOJUYXZQYME-UHFFFAOYSA-N
Formula:	C13H22Cl2O4
SMILES:	CCCCCCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	313.22

Physical Properties

Property code	Value	Unit	Source
gf	-435.56	kJ/mol	Joback Method
hf	-838.01	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.627		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpola	2004.00		NIST Webbook
rinpola	2004.00		NIST Webbook
tb	723.84	K	Joback Method
tc	911.74	K	Joback Method
tf	425.43	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.11	J/molxK	723.84	Joback Method
cpg	640.84	J/molxK	755.16	Joback Method
cpg	653.80	J/molxK	786.47	Joback Method
cpg	666.00	J/molxK	817.79	Joback Method
cpg	677.44	J/molxK	849.10	Joback Method
cpg	688.12	J/molxK	880.42	Joback Method
cpg	698.07	J/molxK	911.74	Joback Method
dvisc	0.0012999	Paxs	425.43	Joback Method

dvisc	0.0006770	Paxs	475.16	Joback Method
dvisc	0.0003990	Paxs	524.90	Joback Method
dvisc	0.0002577	Paxs	574.63	Joback Method
dvisc	0.0001784	Paxs	624.37	Joback Method
dvisc	0.0001304	Paxs	674.10	Joback Method
dvisc	0.0000995	Paxs	723.84	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=U349406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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