

Succinic acid, 2,2-dichloroethyl tetradecyl ester

Inchi:	InChI=1S/C20H36Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-25-19(23)14-15-20(24)26-17
InchiKey:	NFGHDBZFEYGCGM-UHFFFAOYSA-N
Formula:	C20H36Cl2O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	411.40

Physical Properties

Property code	Value	Unit	Source
gf	-376.62	kJ/mol	Joback Method
hf	-982.49	kJ/mol	Joback Method
hfus	58.00	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.358		Crippen Method
mvol	332.020	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	884.00	K	Joback Method
tc	1082.74	K	Joback Method
tf	504.32	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.76	J/molxK	884.00	Joback Method
cpg	1047.19	J/molxK	917.12	Joback Method
cpg	1062.45	J/molxK	950.25	Joback Method
cpg	1076.59	J/molxK	983.37	Joback Method
cpg	1089.62	J/molxK	1016.50	Joback Method
cpg	1101.56	J/molxK	1049.62	Joback Method
cpg	1112.45	J/molxK	1082.74	Joback Method
dvisc	0.0005909	Paxs	504.32	Joback Method

dvisc	0.0002842	Paxs	567.60	Joback Method
dvisc	0.0001583	Paxs	630.88	Joback Method
dvisc	0.0000981	Paxs	694.16	Joback Method
dvisc	0.0000659	Paxs	757.44	Joback Method
dvisc	0.0000470	Paxs	820.72	Joback Method
dvisc	0.0000352	Paxs	884.00	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=U349413&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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