

Succinic acid, 2,2,2-trichloroethyl undecyl ester

Inchi:	InChI=1S/C17H29Cl3O4/c1-2-3-4-5-6-7-8-9-10-13-23-15(21)11-12-16(22)24-14-17(18,19)
InchiKey:	IDHHVODZKZKOPI-UHFFFAOYSA-N
Formula:	C17H29Cl3O4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	403.77

Physical Properties

Property code	Value	Unit	Source
gf	-408.53	kJ/mol	Joback Method
hf	-939.78	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	83.61	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.754		Crippen Method
mcvol	301.990	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinsol	2465.00		NIST Webbook
tb	850.00	K	Joback Method
tc	1047.84	K	Joback Method
tf	517.85	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.37	J/molxK	850.00	Joback Method
cpg	942.37	J/molxK	1014.86	Joback Method
cpg	931.76	J/molxK	981.89	Joback Method
cpg	920.29	J/molxK	948.92	Joback Method
cpg	907.93	J/molxK	915.95	Joback Method
cpg	894.63	J/molxK	882.97	Joback Method
cpg	952.15	J/molxK	1047.84	Joback Method
dvisc	0.0000406	Paxs	850.00	Joback Method
dvisc	0.0000537	Paxs	794.64	Joback Method

dvisc	0.0000740	Paxs	739.28	Joback Method
dvisc	0.0001073	Paxs	683.92	Joback Method
dvisc	0.0001663	Paxs	628.57	Joback Method
dvisc	0.0002806	Paxs	573.21	Joback Method
dvisc	0.0005291	Paxs	517.85	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=U349174&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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