

Succinic acid, tetradecyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C20H35Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-26-18(24)14-15-19(25)27-1
InchiKey:	GDSXXLDWZMMLAH-UHFFFAOYSA-N
Formula:	C20H35Cl3O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	445.85

Physical Properties

Property code	Value	Unit	Source
gf	-383.27	kJ/mol	Joback Method
hf	-1001.70	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.924		Crippen Method
mvol	344.260	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	2761.00		NIST Webbook
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tb	918.64	K	Joback Method
tc	1125.13	K	Joback Method
tf	551.66	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.01	J/molxK	918.64	Joback Method
cpg	1073.34	J/molxK	953.05	Joback Method
cpg	1087.56	J/molxK	987.47	Joback Method
cpg	1100.70	J/molxK	1021.88	Joback Method
cpg	1112.83	J/molxK	1056.30	Joback Method
cpg	1123.99	J/molxK	1090.71	Joback Method
cpg	1134.22	J/molxK	1125.13	Joback Method
dvisc	0.0003588	Paxs	551.66	Joback Method

dvisc	0.0001842	Paxs	612.82	Joback Method
dvisc	0.0001068	Paxs	673.99	Joback Method
dvisc	0.0000677	Paxs	735.15	Joback Method
dvisc	0.0000461	Paxs	796.31	Joback Method
dvisc	0.0000331	Paxs	857.48	Joback Method
dvisc	0.0000249	Paxs	918.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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