

Succinic acid, octyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C14H23Cl3O4/c1-2-3-4-5-6-7-10-20-12(18)8-9-13(19)21-11-14(15,16)17/h2-11
InchiKey:	WZMILCOCAUGKFO-UHFFFAOYSA-N
Formula:	C14H23Cl3O4
SMILES:	CCCCCCCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	361.69

Physical Properties

Property code	Value	Unit	Source
gf	-433.79	kJ/mol	Joback Method
hf	-877.86	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.584		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinqol	2157.00		NIST Webbook
tb	781.36	K	Joback Method
tc	977.33	K	Joback Method
tf	484.04	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.06	J/molxK	781.36	Joback Method
cpg	767.79	J/molxK	944.66	Joback Method
cpg	757.86	J/molxK	912.00	Joback Method
cpg	747.14	J/molxK	879.34	Joback Method
cpg	735.62	J/molxK	846.68	Joback Method
cpg	723.27	J/molxK	814.02	Joback Method
cpg	776.97	J/molxK	977.33	Joback Method
dvisc	0.0000654	Paxs	781.36	Joback Method
dvisc	0.0000857	Paxs	731.81	Joback Method

dvisc	0.0001169	Paxs	682.25	Joback Method
dvisc	0.0001672	Paxs	632.70	Joback Method
dvisc	0.0002542	Paxs	583.15	Joback Method
dvisc	0.0004178	Paxs	533.59	Joback Method
dvisc	0.0007602	Paxs	484.04	Joback Method

Sources

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=U349171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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