Succinic acid, 2-ethylhexyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C14H23Cl3O4/c1-3-5-6-11(4-2)9-20-12(18)7-8-13(19)21-10-14(15,16)17/h11H

InchiKey: XYMVHQUJLLKAES-UHFFFAOYSA-N

Formula: C14H23Cl3O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 361.69

Physical Properties

Property code	Value	Unit	Source
gf	-436.23	kJ/mol	Joback Method
hf	-883.14	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.440		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	780.92	K	Joback Method
tc	979.19	K	Joback Method
tf	469.04	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.63	J/mol×K	780.92	Joback Method
cpg	768.85	J/mol×K	946.15	Joback Method
cpg	758.88	J/mol×K	913.10	Joback Method
cpg	748.09	J/mol×K	880.06	Joback Method
cpg	736.48	J/mol×K	847.01	Joback Method
cpg	724.00	J/mol×K	813.97	Joback Method
cpg	778.05	J/mol×K	979.19	Joback Method
dvisc	0.0000602	Pa×s	780.92	Joback Method

dvisc	0.0000803	Pa×s	728.94	Joback Method
dvisc	0.0001120	Pa×s	676.96	Joback Method
dvisc	0.0001651	Pa×s	624.98	Joback Method
dvisc	0.0002611	Pa×s	573.00	Joback Method
dvisc	0.0004524	Pa×s	521.02	Joback Method
dvisc	0.0008856	Pa×s	469.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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