Succinic acid, isohexyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H19Cl3O4/c1-9(2)4-3-7-18-10(16)5-6-11(17)19-8-12(13,14)15/h9H,3-8H2,

InchiKey: ZFKJXSGRVYKTJB-UHFFFAOYSA-N

Formula: C12H19Cl3O4

SMILES: CC(C)CCCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 333.64

Physical Properties

Property code	Value	Unit	Source
gf	-453.07	kJ/mol	Joback Method
hf	-841.86	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.659		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	735.16	K	Joback Method
tc	935.81	K	Joback Method
tf	446.50	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.09	J/mol×K	735.16	Joback Method
cpg	614.67	J/mol×K	768.60	Joback Method
cpg	626.42	J/mol×K	802.04	Joback Method
cpg	637.37	J/mol×K	835.49	Joback Method
cpg	647.53	J/mol×K	868.93	Joback Method
cpg	656.94	J/mol×K	902.37	Joback Method
cpg	665.61	J/mol×K	935.81	Joback Method
dvisc	0.0011206	Pa×s	446.50	Joback Method

dvisc	0.0005868	Pa×s	494.61	Joback Method
dvisc	0.0003447	Pa×s	542.72	Joback Method
dvisc	0.0002208	Pa×s	590.83	Joback Method
dvisc	0.0001512	Pa×s	638.94	Joback Method
dvisc	0.0001092	Pa×s	687.05	Joback Method
dvisc	0.0000823	Pa×s	735.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349169&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