Succinic acid, isobutyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H15Cl3O4/c1-7(2)5-16-8(14)3-4-9(15)17-6-10(11,12)13/h7H,3-6H2,1-2H3
InchiKey: MGZOIMXKEQGDAC-UHFFFAOYSA-N
Formula: C10H15Cl3O4
SMILES: CC(C)COC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 305.58

Physical Properties

Property code	Value	Unit	Source
gf	-469.91	kJ/mol	Joback Method
hf	-800.58	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	67.64	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.879		Crippen Method
mcvol	203.360	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	689.40	K	Joback Method
tc	894.40	K	Joback Method
tf	423.96	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.24	J/mol×K	689.40	Joback Method
cpg	509.82	J/mol×K	723.57	Joback Method
cpg	520.63	J/mol×K	757.73	Joback Method
cpg	530.71	J/mol×K	791.90	Joback Method
cpg	540.06	J/mol×K	826.07	Joback Method
cpg	548.70	J/mol×K	860.23	Joback Method
cpg	556.65	J/mol×K	894.40	Joback Method
dvisc	0.0013957	Pa×s	423.96	Joback Method

dvisc	0.0007509	Pa×s	468.20	Joback Method
dvisc	0.0004497	Pa×s	512.44	Joback Method
dvisc	0.0002922	Pa×s	556.68	Joback Method
dvisc	0.0002023	Pa×s	600.92	Joback Method
dvisc	0.0001473	Pa×s	645.16	Joback Method
dvisc	0.0001117	Pa×s	689.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349166&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

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