Succinic acid, hept-2-yl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C13H21Cl3O4/c1-3-4-5-6-10(2)20-12(18)8-7-11(17)19-9-13(14,15)16/h10H,3-9

InchiKey: KKYWMSYAEHWDHA-UHFFFAOYSA-N

Formula: C13H21Cl3O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 347.66

Physical Properties

Property code	Value	Unit	Source
gf	-444.65	kJ/mol	Joback Method
hf	-862.50	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.192		Crippen Method
mcvol	245.630	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	758.04	K	Joback Method
tc	957.24	K	Joback Method
tf	457.77	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.81	J/mol×K	758.04	Joback Method
cpg	712.45	J/mol×K	924.04	Joback Method
cpg	702.74	J/mol×K	890.84	Joback Method
cpg	692.24	J/mol×K	857.64	Joback Method
cpg	680.94	J/mol×K	824.44	Joback Method
cpg	668.81	J/mol×K	791.24	Joback Method
cpg	721.41	J/mol×K	957.24	Joback Method
dvisc	0.0000705	Pa×s	758.04	Joback Method

dvisc	0.0000937	Pa×s	707.99	Joback Method
dvisc	0.0001303	Pa×s	657.95	Joback Method
dvisc	0.0001911	Pa×s	607.90	Joback Method
dvisc	0.0003004	Pa×s	557.86	Joback Method
dvisc	0.0005161	Pa×s	507.81	Joback Method
dvisc	0.0009980	Pa×s	457.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390234&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