Succinic acid, cyclohexylmethyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C13H19Cl3O4/c14-13(15,16)9-20-12(18)7-6-11(17)19-8-10-4-2-1-3-5-10/h10H

InchiKey: BRZJJHSFYXYVSL-UHFFFAOYSA-N

Formula: C13H19Cl3O4

SMILES: O=C(CCC(=O)OCC(Cl)(Cl)Cl)OCC1CCCCC1

Mol. weight [g/mol]: 345.65

Physical Properties

Property code	Value	Unit	Source
gf	-417.76	kJ/mol	Joback Method
hf	-802.90	kJ/mol	Joback Method
hfus	32.01	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.803		Crippen Method
mcvol	234.770	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	778.03	K	Joback Method
tc	999.99	K	Joback Method
tf	480.15	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.86	J/mol×K	778.03	Joback Method
cpg	707.70	J/mol×K	963.00	Joback Method
cpg	697.95	J/mol×K	926.00	Joback Method
cpg	687.14	J/mol×K	889.01	Joback Method
cpg	675.21	J/mol×K	852.02	Joback Method
cpg	662.12	J/mol×K	815.02	Joback Method
cpg	716.40	J/mol×K	999.99	Joback Method
dvisc	0.0000787	Pa×s	778.03	Joback Method

dvisc	0.0001037	Pa×s	728.38	Joback Method
dvisc	0.0001423	Pa×s	678.74	Joback Method
dvisc	0.0002052	Pa×s	629.09	Joback Method
dvisc	0.0003151	Pa×s	579.44	Joback Method
dvisc	0.0005244	Pa×s	529.80	Joback Method
dvisc	0.0009698	Pa×s	480.15	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=U390237&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