Carbonic acid, 2,2,2-trichloroethyl cyclohexyl ester

Inchi: InChI=1S/C9H13Cl3O3/c10-9(11,12)6-14-8(13)15-7-4-2-1-3-5-7/h7H,1-6H2
InchiKey: MDNHFAMHCYNWIL-UHFFFAOYSA-N
Formula: C9H13Cl3O3
SMILES: O=C(OCC(Cl)(Cl)Cl)OC1CCCCC1
Mol. weight [g/mol]: 275.56

Physical Properties

Property code	Value	Unit	Source
gf	-322.52	kJ/mol	Joback Method
hf	-607.76	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	59.48	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.842		Crippen Method
mcvol	176.840	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	632.64	K	Joback Method
tc	864.53	K	Joback Method
tf	385.14	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.98	J/mol×K	632.64	Joback Method
cpg	437.63	J/mol×K	671.29	Joback Method
cpg	451.19	J/mol×K	709.94	Joback Method
cpg	463.68	J/mol×K	748.58	Joback Method
cpg	475.14	J/mol×K	787.23	Joback Method
cpg	485.60	J/mol×K	825.88	Joback Method
cpg	495.07	J/mol×K	864.53	Joback Method
dvisc	0.0019954	Pa×s	385.14	Joback Method
dvisc	0.0010577	Pa×s	426.39	Joback Method

dvisc	0.0006271	Pa×s	467.64	Joback Method
dvisc	0.0004047	Pa×s	508.89	Joback Method
dvisc	0.0002789	Pa×s	550.14	Joback Method
dvisc	0.0002024	Pa×s	591.39	Joback Method
dvisc	0.0001532	Pa×s	632.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357895&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