Carbonic acid, 2,2,2-trichloroethyl isopropyl ester

Inchi: InChI=1S/C6H9Cl3O3/c1-4(2)12-5(10)11-3-6(7,8)9/h4H,3H2,1-2H3
InchiKey: BXVZTZVGXVIVBP-UHFFFAOYSA-N
Formula: C6H9Cl3O3
SMILES: CC(C)OC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 235.49

Physical Properties

Property code	Value	Unit	Source
gf	-374.67	kJ/mol	Joback Method
hf	-605.44	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.918		Crippen Method
mcvol	145.430	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1206.00		NIST Webbook
tb	544.01	K	Joback Method
tc	754.31	K	Joback Method
tf	328.95	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.45	J/mol×K	544.01	Joback Method
cpg	307.07	J/mol×K	579.06	Joback Method
cpg	316.13	J/mol×K	614.11	Joback Method
cpg	324.64	J/mol×K	649.16	Joback Method
cpg	332.61	J/mol×K	684.21	Joback Method
cpg	340.05	J/mol×K	719.26	Joback Method
cpg	346.97	J/mol×K	754.31	Joback Method
dvisc	0.0027759	Pa×s	328.95	Joback Method
dvisc	0.0014570	Pa×s	364.79	Joback Method

dvisc	0.0008582	Pa×s	400.64	Joback Method
dvisc	0.0005514	Pa×s	436.48	Joback Method
dvisc	0.0003789	Pa×s	472.32	Joback Method
dvisc	0.0002745	Pa×s	508.17	Joback Method
dvisc	0.0002075	Pa×s	544.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357892&Units=SI

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