Carbonic acid, 2,2,2-trichloroethyl neopentyl ester

Inchi: InChI=1S/C8H13Cl3O3/c1-7(2,3)4-13-6(12)14-5-8(9,10)11/h4-5H2,1-3H3
InchiKey: DGZGZIOPBXWWDS-UHFFFAOYSA-N
Formula: C8H13Cl3O3
SMILES: CC(C)(C)COC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 263.55

Physical Properties

Property code	Value	Unit	Source
gf	-352.55	kJ/mol	Joback Method
hf	-650.19	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.556		Crippen Method
mcvol	173.610	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
tb	586.98	K	Joback Method
tc	798.54	K	Joback Method
tf	368.91	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.35	J/mol×K	586.98	Joback Method
cpg	441.77	J/mol×K	763.28	Joback Method
cpg	432.94	J/mol×K	728.02	Joback Method
cpg	423.42	J/mol×K	692.76	Joback Method
cpg	413.17	J/mol×K	657.50	Joback Method
cpg	402.16	J/mol×K	622.24	Joback Method
cpg	449.94	J/mol×K	798.54	Joback Method
dvisc	0.0001523	Pa×s	586.98	Joback Method

dvisc	0.0002028	Pa×s	550.63	Joback Method
dvisc	0.0002813	Pa×s	514.29	Joback Method
dvisc	0.0004100	Pa×s	477.95	Joback Method
dvisc	0.0006360	Pa×s	441.60	Joback Method
dvisc	0.0010673	Pa×s	405.25	Joback Method
dvisc	0.0019835	Pa×s	368.91	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=U357893&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