Cyclooctene, 1-trichloromethyl

Inchi: InChI=1S/C9H13Cl3/c10-9(11,12)8-6-4-2-1-3-5-7-8/h6H,1-5,7H2/b8-6+
InchiKey: FCFMGYWICYEEAL-SOFGYWHQSA-N
Formula: C9H13Cl3
SMILES: ClC(Cl)(Cl)C1=CCCCCCC1
Mol. weight [g/mol]: 227.56

Physical Properties

Property code	Value	Unit	Source
gf	20.24	kJ/mol	Joback Method
hf	-176.41	kJ/mol	Joback Method
hfus	11.64	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.637		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	551.28	K	Joback Method
tc	803.72	K	Joback Method
tf	301.23	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.00	J/mol×K	551.28	Joback Method
cpg	352.25	J/mol×K	593.35	Joback Method
cpg	368.11	J/mol×K	635.43	Joback Method
cpg	382.65	J/mol×K	677.50	Joback Method
cpg	395.94	J/mol×K	719.58	Joback Method
cpg	408.04	J/mol×K	761.65	Joback Method
cpg	419.04	J/mol×K	803.72	Joback Method
dvisc	0.0069043	Pa×s	301.23	Joback Method

dvisc	0.0024538	Pa×s	342.91	Joback Method
dvisc	0.0010913	Pa×s	384.58	Joback Method
dvisc	0.0005686	Pa×s	426.25	Joback Method
dvisc	0.0003328	Pa×s	467.93	Joback Method
dvisc	0.0002126	Pa×s	509.60	Joback Method
dvisc	0.0001453	Pa×s	551.28	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=R515325&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