

Cyclooctane, 1-chloro-2-(trichloromethyl)

Inchi:	InChI=1S/C9H14Cl4/c10-8-6-4-2-1-3-5-7(8)9(11,12)13/h7-8H,1-6H2
InchiKey:	FYKGBQOLMOWDP-UHFFFAOYSA-N
Formula:	C9H14Cl4
SMILES:	C1C(C(C(C(C1)Cl)Cl)Cl)Cl
Mol. weight [g/mol]:	264.02

Physical Properties

Property code	Value	Unit	Source
gf	-27.44	kJ/mol	Joback Method
hf	-279.14	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.934		Crippen Method
mvol	175.770	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1707.00		NIST Webbook
tb	575.23	K	Joback Method
tc	828.00	K	Joback Method
tf	309.39	K	Joback Method
vc	0.640	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.98	J/molxK	575.23	Joback Method
cpg	404.71	J/molxK	617.36	Joback Method
cpg	421.94	J/molxK	659.49	Joback Method
cpg	437.74	J/molxK	701.61	Joback Method
cpg	452.16	J/molxK	743.74	Joback Method
cpg	465.27	J/molxK	785.87	Joback Method
cpg	477.10	J/molxK	828.00	Joback Method
dvisc	0.0058243	Paxs	309.39	Joback Method

dvisc	0.0022157	Paxs	353.70	Joback Method
dvisc	0.0010453	Paxs	398.00	Joback Method
dvisc	0.0005732	Paxs	442.31	Joback Method
dvisc	0.0003507	Paxs	486.62	Joback Method
dvisc	0.0002329	Paxs	530.92	Joback Method
dvisc	0.0001647	Paxs	575.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R515310&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

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