

Cyclooctene, 3-trichloromethyl

Inchi:	InChI=1S/C9H13Cl3/c10-9(11,12)8-6-4-2-1-3-5-7-8/h4,6,8H,1-3,5,7H2/b6-4+
InchiKey:	SXAVYDLPOKHCML-GQCTYLIASA-N
Formula:	C9H13Cl3
SMILES:	C1C(Cl)(Cl)C1C=CCCCC1
Mol. weight [g/mol]:	227.56

Physical Properties

Property code	Value	Unit	Source
gf	22.16	kJ/mol	Joback Method
hf	-185.28	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.493		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	541.63	K	Joback Method
tc	792.94	K	Joback Method
tf	284.47	K	Joback Method
vc	0.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.42	J/mol×K	541.63	Joback Method
cpg	354.62	J/mol×K	583.51	Joback Method
cpg	371.37	J/mol×K	625.40	Joback Method
cpg	386.73	J/mol×K	667.28	Joback Method
cpg	400.78	J/mol×K	709.17	Joback Method
cpg	413.56	J/mol×K	751.05	Joback Method
cpg	425.16	J/mol×K	792.94	Joback Method
dvisc	0.0088298	Paxs	284.47	Joback Method

dvisc	0.0029693	Paxs	327.33	Joback Method
dvisc	0.0012852	Paxs	370.19	Joback Method
dvisc	0.0006618	Paxs	413.05	Joback Method
dvisc	0.0003861	Paxs	455.91	Joback Method
dvisc	0.0002471	Paxs	498.77	Joback Method
dvisc	0.0001697	Paxs	541.63	Joback Method

Sources

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=R515330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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