

Cyclooctane, 1-bromo-2-(trichloromethyl)

Inchi: InChI=1S/C9H14BrCl3/c10-8-6-4-2-1-3-5-7(8)9(11,12)13/h7-8H,1-6H2
InchiKey: WATALFRMBMIIB-UHFFFAOYSA-N
Formula: C9H14BrCl3
SMILES: ClC(Cl)(Cl)C1CCCCC1Br
Mol. weight [g/mol]: 308.47

Physical Properties

Property code	Value	Unit	Source
gf	-1.19	kJ/mol	Joback Method
hf	-237.07	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	54.39	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.091		Crippen Method
mvol	181.030	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	603.96	K	Joback Method
tc	866.92	K	Joback Method
tf	339.27	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.11	J/molxK	603.96	Joback Method
cpg	476.38	J/molxK	823.09	Joback Method
cpg	463.97	J/molxK	779.27	Joback Method
cpg	450.22	J/molxK	735.44	Joback Method
cpg	435.04	J/molxK	691.61	Joback Method
cpg	418.36	J/molxK	647.79	Joback Method
cpg	487.51	J/molxK	866.92	Joback Method
dvisc	0.0001524	Paxs	603.96	Joback Method

dvisc	0.0002111	Paxs	559.85	Joback Method
dvisc	0.0003094	Paxs	515.73	Joback Method
dvisc	0.0004869	Paxs	471.62	Joback Method
dvisc	0.0008415	Paxs	427.50	Joback Method
dvisc	0.0016496	Paxs	383.38	Joback Method
dvisc	0.0038519	Paxs	339.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515305&Units=SI
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

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
mccvol:	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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