Oxetane, 3-bromomethyl-3-chloromethyl

Inchi: InChI=1S/C5H8BrClO/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: WHFZYXGDOQLICS-UHFFFAOYSA-N
Formula: C5H8BrClO
SMILES: ClCC1(CBr)COC1
Mol. weight [g/mol]: 199.47

Physical Properties

Property code	Value	Unit	Source
gf	-49.35	kJ/mol	Joback Method
hf	-186.06	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	40.99	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.637		Crippen Method
mcvol	106.060	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
rinpol	1155.00		NIST Webbook
tb	455.59	K	Joback Method
tc	682.93	K	Joback Method
tf	300.72	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.28	J/mol×K	455.59	Joback Method
cpg	204.82	J/mol×K	493.48	Joback Method
cpg	214.32	J/mol×K	531.37	Joback Method
cpg	222.91	J/mol×K	569.26	Joback Method
cpg	230.74	J/mol×K	607.15	Joback Method
cpg	237.96	J/mol×K	645.04	Joback Method
cpg	244.72	J/mol×K	682.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R6638&Units=SI

Legend

cpg:	Ideal gas heat capacity
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