Oxetane, 3-bromomethyl-3-iodomethyl

Inchi: InChI=1S/C5H8BrIO/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: FNEOLQRYEPFPEV-UHFFFAOYSA-N
Formula: C5H8BrIO
SMILES: BrCC1(CI)COC1
Mol. weight [g/mol]: 290.93

Physical Properties

Property code	Value	Unit	Source
gf	20.70	kJ/mol	Joback Method
hf	-93.45	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.833		Crippen Method
mcvol	119.640	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	511.30	K	Joback Method
tc	769.75	K	Joback Method
tf	328.86	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.86	J/mol×K	511.30	Joback Method
cpg	222.80	J/mol×K	554.38	Joback Method
cpg	231.65	J/mol×K	597.45	Joback Method
cpg	239.65	J/mol×K	640.53	Joback Method
cpg	247.01	J/mol×K	683.60	Joback Method
cpg	253.98	J/mol×K	726.68	Joback Method
cpg	260.78	J/mol×K	769.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6654&Units=SI
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

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