Oxetane, 3-bromomethyl-3-hydroxymethyl

Inchi: InChI=1S/C5H9BrO2/c6-1-5(2-7)3-8-4-5/h7H,1-4H2
InchiKey: SESXZSLSTRITGO-UHFFFAOYSA-N
Formula: C5H9BrO2
SMILES: OCC1(CBr)COC1
Mol. weight [g/mol]: 181.03

Physical Properties

Property code	Value	Unit	Source
gf	-174.24	kJ/mol	Joback Method
hf	-322.55	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.390		Crippen Method
mcvol	99.690	ml/mol	McGowan Method
pc	5519.63	kPa	Joback Method
rinpol	1220.00		NIST Webbook
tb	510.34	K	Joback Method
tc	716.48	K	Joback Method
tf	331.62	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.95	J/mol×K	510.34	Joback Method
cpg	221.81	J/mol×K	544.70	Joback Method
cpg	229.95	J/mol×K	579.05	Joback Method
cpg	237.48	J/mol×K	613.41	Joback Method
cpg	244.50	J/mol×K	647.77	Joback Method
cpg	251.13	J/mol×K	682.13	Joback Method
cpg	257.48	J/mol×K	716.48	Joback Method

Sources

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=R6641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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