3-Bromo-3-methyldiazirine

Inchi: InChI=1S/C2H3BrN2/c1-2(3)4-5-2/h1H3
InchiKey: SWGOAGINOJLLAU-UHFFFAOYSA-N
Formula: C2H3BrN2
SMILES: CC1(Br)N=N1
Mol. weight [g/mol]: 134.96
CAS: 4222-23-5

Physical Properties

Property code	Value	Unit	Source
gf	299.06	kJ/mol	Joback Method
hf	229.48	kJ/mol	Joback Method
hfus	9.56	kJ/mol	Joback Method
hvap	37.95	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.521		Crippen Method
mcvol	61.340	ml/mol	McGowan Method
pc	7859.26	kPa	Joback Method
tb	424.86	K	Joback Method
tc	675.95	K	Joback Method
tf	357.78	K	Joback Method
vc	0.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.37	J/mol×K	424.86	Joback Method
cpg	121.38	J/mol×K	466.71	Joback Method
cpg	129.37	J/mol×K	508.56	Joback Method
cpg	136.50	J/mol×K	550.41	Joback Method
cpg	142.90	J/mol×K	592.25	Joback Method
cpg	148.72	J/mol×K	634.10	Joback Method
cpg	154.10	J/mol×K	675.95	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=C4222235&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume