Bicyclo[2.2.2]octane, 1-bromo-

Other names: 1-Bromobicyclo[2.2.2]octane
Inchi: InChI=1S/C8H13Br/c9-8-4-1-7(2-5-8)3-6-8/h7H,1-6H2
InchiKey: GKIJLFQCRFWQCZ-UHFFFAOYSA-N
Formula: C8H13Br
SMILES: BrC12CCC(CC1)CC2
Mol. weight [g/mol]: 189.09
CAS: 7697-09-8

Physical Properties

Property code	Value	Unit	Source
gf	122.61	kJ/mol	Joback Method
hf	-33.60	kJ/mol	Joback Method
hfus	7.53	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
ie	9.67	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	3.104		Crippen Method
mcvol	119.360	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	470.86	K	Joback Method
tc	710.72	K	Joback Method
tf	292.46	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.97	J/mol×K	470.86	Joback Method
cpg	264.55	J/mol×K	510.84	Joback Method
cpg	280.49	J/mol×K	550.81	Joback Method
cpg	295.00	J/mol×K	590.79	Joback Method
cpg	308.31	J/mol×K	630.76	Joback Method
cpg	320.61	J/mol×K	670.74	Joback Method

cpg	332.12	J/mol×K	710.72	Joback Method

Sources

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=C7697098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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

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