

Bicyclo[6.1.0]nonane, 9,9-dibromo-

Other names:	9,9-Dibromobicyclo[6.1.0]nonane
Inchi:	InChI=1S/C9H14Br2/c10-9(11)7-5-3-1-2-4-6-8(7)/h7-8H,1-6H2
InchiKey:	UDZVXFNKFQAZEC-UHFFFAOYSA-N
Formula:	C9H14Br2
SMILES:	BrC1(Br)C2CCCCCCC21
Mol. weight [g/mol]:	282.01
CAS:	1196-95-8

Physical Properties

Property code	Value	Unit	Source
gf	125.54	kJ/mol	Joback Method
hf	-54.41	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	47.38	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.073		Crippen Method
mcvol	150.950	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	559.50	K	Joback Method
tc	820.51	K	Joback Method
tf	355.77	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.55	J/molxK	559.50	Joback Method
cpg	354.46	J/molxK	603.00	Joback Method
cpg	370.83	J/molxK	646.50	Joback Method
cpg	385.94	J/molxK	690.00	Joback Method
cpg	400.05	J/molxK	733.50	Joback Method
cpg	413.43	J/molxK	777.00	Joback Method
cpg	426.35	J/molxK	820.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1196958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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

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