

Bicyclo[3.3.1]nonan-2-one

Inchi:	InChI=1S/C9H14O/c10-9-5-4-7-2-1-3-8(9)6-7/h7-8H,1-6H2
InchiKey:	JTYKTCBMGNIYBC-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	O=C1CCC2CCCC1C2
Mol. weight [g/mol]:	138.21
CAS:	2568-17-4

Physical Properties

Property code	Value	Unit	Source
gf	-12.49	kJ/mol	Joback Method
hf	-239.67	kJ/mol	Joback Method
hfus	8.55	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
ie	8.94	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.156		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	499.43	K	Joback Method
tc	734.32	K	Joback Method
tf	284.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.47	J/mol×K	499.43	Joback Method
cpg	296.85	J/mol×K	538.58	Joback Method
cpg	315.07	J/mol×K	577.73	Joback Method
cpg	332.18	J/mol×K	616.87	Joback Method
cpg	348.20	J/mol×K	656.02	Joback Method
cpg	363.18	J/mol×K	695.17	Joback Method
cpg	377.14	J/mol×K	734.32	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=C2568174&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
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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