Bicyclo[3.2.1]octan-3-one

Other names: 3-Bicyclo[3.2.1]octanone
Inchi: InChI=1S/C8H12O/c9-8-4-6-1-2-7(3-6)5-8/h6-7H,1-5H2
InchiKey: HIMMOVPGAJKVOS-UHFFFAOYSA-N
Formula: C8H12O
SMILES: O=C1CC2CCC(C1)C2
Mol. weight [g/mol]: 124.18
CAS: 14252-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-8.81	kJ/mol	Joback Method
hf	-221.00 ± 8.40	kJ/mol	NIST Webbook
hfus	8.06	kJ/mol	Joback Method
hvap	37.82	kJ/mol	Joback Method
ie	9.23	eV	NIST Webbook
log10ws	-1.76		Crippen Method
logp	1.766		Crippen Method
mcvol	103.430	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	472.28	K	Joback Method
tc	702.14	K	Joback Method
tf	276.98	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.73	J/mol×K	472.28	Joback Method
cpg	250.02	J/mol×K	510.59	Joback Method
cpg	266.30	J/mol×K	548.90	Joback Method
cpg	281.60	J/mol×K	587.21	Joback Method
cpg	295.95	J/mol×K	625.52	Joback Method
cpg	309.40	J/mol×K	663.83	Joback Method
cpg	321.98	J/mol×K	702.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14252052&Units=SI
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

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