

Bicyclo[2.2.2]octanone

Other names:	Bicyclo[2.2.2]octan-2-one
Inchi:	InChI=1S/C8H12O/c9-8-5-6-1-3-7(8)4-2-6/h6-7H,1-5H2
InchiKey:	VEPYQCZRVLNDBC-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	O=C1CC2CCC1CC2
Mol. weight [g/mol]:	124.18
CAS:	2716-23-6

Physical Properties

Property code	Value	Unit	Source
chl	-4589.00	kJ/mol	NIST Webbook
gf	-8.81	kJ/mol	Joback Method
hf	-218.00 ± 8.40	kJ/mol	NIST Webbook
hf	-222.00 ± 5.40	kJ/mol	NIST Webbook
hfl	-274.00 ± 4.60	kJ/mol	NIST Webbook
hfus	8.06	kJ/mol	Joback Method
hvap	52.00 ± 2.00	kJ/mol	NIST Webbook
ie	9.07 ± 0.05	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.80	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

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=C2716236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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