Bicyclo[3.3.1]nonan-9-one

Other names: Bicyclo[3.3.1]nona-9-one
Inchi: InChI=1S/C9H14O/c10-9-7-3-1-4-8(9)6-2-5-7/h7-8H,1-6H2
InchiKey: SKTMMSQPXGWCAP-UHFFFAOYSA-N
Formula: C9H14O
SMILES: O=C1C2CCCC1CCC2
Mol. weight [g/mol]: 138.21
CAS: 17931-55-4

Physical Properties

Property code	Value	Unit	Source
gf	-12.49	kJ/mol	Joback Method
hf	-240.00 ± 8.40	kJ/mol	NIST Webbook
hfus	8.55	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
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
hfust	14.11	kJ/mol	300.50	NIST Webbook

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=C17931554&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	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