Bicyclo[3.3.1]non-3-en-2-one

Inchi: InChI=1S/C9H12O/c10-9-5-4-7-2-1-3-8(9)6-7/h4-5,7-8H,1-3,6H2
InchiKey: TUQWWBMBVKVORD-UHFFFAOYSA-N
Formula: C9H12O
SMILES: O=C1C=CC2CCCC1C2
Mol. weight [g/mol]: 136.19
CAS: 10036-12-1

Physical Properties

Property code	Value	Unit	Source
gf	17.47	kJ/mol	Joback Method
hf	-181.89	kJ/mol	Joback Method
hfus	9.77	kJ/mol	Joback Method
hvap	40.51	kJ/mol	Joback Method
ie	9.01	eV	NIST Webbook
log10ws	-2.03		Crippen Method
logp	1.932		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	498.59	K	Joback Method
tc	735.98	K	Joback Method
tf	285.49	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.59	J/mol×K	498.59	Joback Method
cpg	278.62	J/mol×K	538.15	Joback Method
cpg	295.55	J/mol×K	577.72	Joback Method
cpg	311.40	J/mol×K	617.28	Joback Method
cpg	326.21	J/mol×K	656.85	Joback Method
cpg	340.01	J/mol×K	696.41	Joback Method
cpg	352.84	J/mol×K	735.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10036121&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

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