1-{Bicyclo[2.2.1]heptan-2-yl}ethanone

Other names: Methyl norbornyl ketone
Inchi: InChI=1S/C9H14O/c1-6(10)9-5-7-2-3-8(9)4-7/h7-9H,2-5H2,1H3
InchiKey: NDZIFIKZHLSCFR-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC(=O)C1CC2CCC1C2
Mol. weight [g/mol]: 138.21
CAS: 109583-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-2.33	kJ/mol	Joback Method
hf	-222.57	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1078.00		NIST Webbook
tb	472.27	K	Joback Method
tc	682.83	K	Joback Method
tf	269.24	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.96	J/mol×K	472.27	Joback Method
cpg	286.18	J/mol×K	507.36	Joback Method
cpg	302.31	J/mol×K	542.46	Joback Method
cpg	317.42	J/mol×K	577.55	Joback Method
cpg	331.56	J/mol×K	612.65	Joback Method
cpg	344.80	J/mol×K	647.74	Joback Method
cpg	357.19	J/mol×K	682.83	Joback Method

dvisc	0.0014655	Pa×s	269.24	Joback Method
dvisc	0.0012738	Pa×s	303.08	Joback Method
dvisc	0.0011388	Pa×s	336.92	Joback Method
dvisc	0.0010391	Pa×s	370.75	Joback Method
dvisc	0.0009628	Pa×s	404.59	Joback Method
dvisc	0.0009027	Pa×s	438.43	Joback Method
dvisc	0.0008542	Pa×s	472.27	Joback Method

Sources

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=C109583348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume