Bicyclo[2.2.1]heptan-2-one, 1-methyl

Inchi: InChI=1S/C8H12O/c1-8-3-2-6(5-8)4-7(8)9/h6H,2-5H2,1H3
InchiKey: ZYVCBPCUGIGFJA-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC12CCC(CC1=O)C2
Mol. weight [g/mol]: 124.18
CAS: 10218-04-9

Physical Properties

Property code	Value	Unit	Source
gf	-2.20	kJ/mol	Joback Method
hf	-191.47	kJ/mol	Joback Method
hfus	3.86	kJ/mol	Joback Method
hvap	36.50	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.766		Crippen Method
mcvol	103.430	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	468.25	K	Joback Method
tc	699.24	K	Joback Method
tf	304.40	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.88	J/mol×K	468.25	Joback Method
cpg	250.25	J/mol×K	506.75	Joback Method
cpg	265.34	J/mol×K	545.25	Joback Method
cpg	279.32	J/mol×K	583.74	Joback Method
cpg	292.33	J/mol×K	622.24	Joback Method
cpg	304.52	J/mol×K	660.74	Joback Method
cpg	316.03	J/mol×K	699.24	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=C10218049&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
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