Bicyclo[3.1.0]hexan-2-one, 1-methyl-4-(1-methylethyl)

Inchi: InChI=1S/C10H16O/c1-7(2)10-5-4-8(11)9(10,3)6-10/h7H,4-6H2,1-3H3
InchiKey: XTUMSZDBTLUZKV-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)C12CCC(=O)C1(C)C2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	18.81	kJ/mol	Joback Method
hf	-216.63	kJ/mol	Joback Method
hfus	1.32	kJ/mol	Joback Method
hvap	39.24	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
tb	509.54	K	Joback Method
tc	739.15	K	Joback Method
tf	339.36	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.53	J/mol×K	509.54	Joback Method
cpg	340.81	J/mol×K	547.81	Joback Method
cpg	356.66	J/mol×K	586.08	Joback Method
cpg	371.34	J/mol×K	624.35	Joback Method
cpg	385.12	J/mol×K	662.61	Joback Method
cpg	398.26	J/mol×K	700.88	Joback Method
cpg	411.04	J/mol×K	739.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324659&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume