Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-

Other names:	«beta»-Pinone
	Nopinon
	Nopinone
	2-Norpinanone, 6,6-dimethyl-
	6,6-Dimethylbicyclo(3.1.1)heptan-2-one
	nopinonee
Inchi:	InChI=1S/C9H14O/c1-9(2)6-3-4-8(10)7(9)5-6/h6-7H,3-5H2,1-2H3
InchiKey:	XZFDKWMYCUEKSS-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1(C)C2CCC(=O)C1C2
Mol. weight [g/mol]:	138.21
CAS:	24903-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-1.49	kJ/mol	Joback Method
hf	-232.45	kJ/mol	Joback Method
hfus	7.52	kJ/mol	Joback Method
hvap	38.41	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1145.00		NIST Webbook

rinpol	1120.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1111.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1577.00		NIST Webbook
tb	486.46	K	Joback Method
tc	713.39	K	Joback Method
tf	311.43	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.51	J/mol×K	486.46	Joback Method
cpg	296.15	J/mol×K	524.28	Joback Method
cpg	312.56	J/mol×K	562.10	Joback Method
cpg	327.88	J/mol×K	599.93	Joback Method
cpg	342.24	J/mol×K	637.75	Joback Method
cpg	355.78	J/mol×K	675.57	Joback Method
cpg	368.63	J/mol×K	713.39	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=C24903955&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume