Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-

Other names: (1R)-(+)-Nopinone
6,6-Dimethylbicyclo[3.1.1]heptan-2-one-, (1R)-
(+)-Nopinone
(1R)-(+)-Norinone

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: 38651-65-9

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	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1142.40		NIST Webbook
rinpol	1152.40		NIST Webbook
tb	482.20	K	NIST Webbook
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

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=C38651659&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume