

Bicyclo[2.2.1]heptan-2-one, 3,3-dimethyl-

Other names:	2-Norbornanone, 3,3-dimethyl- Camphenilone 3,3-Dimethylnorcamphor 3,3-Dimethylbicyclo[2.2.1]heptan-2-one
Inchi:	InChI=1S/C9H14O/c1-9(2)7-4-3-6(5-7)8(9)10/h6-7H,3-5H2,1-2H3
InchiKey:	ZYPYEBYNXWUCEA-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1(C)C(=O)C2CCC1C2
Mol. weight [g/mol]:	138.21
CAS:	13211-15-9

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
ie	8.89	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	2.012		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1085.00		NIST Webbook

rinpol	1086.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1456.00		NIST Webbook
tb	486.46	K	Joback Method
tc	713.39	K	Joback Method
tf	311.43	K	Joback Method
vc	0.450	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13211159&Units=SI
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

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
ie:	Ionization energy
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

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