

Bicyclo[2.2.1]heptan-2-one, 1,4,7,7-tetramethyl-

Other names:	1,4,7,7-Tetramethylbicyclo[2.2.1]heptan-2-one 4-Methylcamphor 2-Norbornanone, 1,4,7,7-tetramethyl-
Inchi:	InChI=1S/C11H18O/c1-9(2)10(3)5-6-11(9,4)8(12)7-10/h5-7H2,1-4H3
InchiKey:	WHTUSNIUKHUYQX-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	CC12CCC(C)(C(=O)C1)C2(C)C
Mol. weight [g/mol]:	166.26
CAS:	10309-50-9

Physical Properties

Property code	Value	Unit	Source
affp	863.30	kJ/mol	NIST Webbook
basg	831.40	kJ/mol	NIST Webbook
gf	4.37	kJ/mol	Joback Method
hf	-243.25	kJ/mol	Joback Method
hfus	0.10	kJ/mol	Joback Method
hvap	40.56	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.792		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	532.70	K	Joback Method
tc	771.24	K	Joback Method
tf	381.77	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.88	J/mol×K	532.70	Joback Method
cpg	389.59	J/mol×K	572.46	Joback Method
cpg	406.79	J/mol×K	612.21	Joback Method
cpg	422.87	J/mol×K	651.97	Joback Method

cpg	438.23	J/mol×K	691.72	Joback Method
cpg	453.24	J/mol×K	731.48	Joback Method
cpg	468.32	J/mol×K	771.24	Joback Method

Sources

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=C10309509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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