

3-Methylene-2-norbornanone

Other names:	Bicyclo[2.2.1]heptan-2-one, 3-methylene-2-Norbornanone, 3-methylene-3-methylenenorbornan-2-one
Inchi:	InChI=1S/C8H10O/c1-5-6-2-3-7(4-6)8(5)9/h6-7H,1-4H2
InchiKey:	FNOOZJAPZFHNCW-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	C=C1C(=O)C2CCC1C2
Mol. weight [g/mol]:	122.16
CAS:	5597-27-3

Physical Properties

Property code	Value	Unit	Source
gf	56.37	kJ/mol	Joback Method
hf	-122.47	kJ/mol	Joback Method
hfus	9.00	kJ/mol	Joback Method
hvap	37.81	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.542		Crippen Method
mcvol	99.130	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	467.17	K	Joback Method
tc	690.21	K	Joback Method
tf	294.18	K	Joback Method
vc	0.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.46	J/mol×K	467.17	Joback Method
cpg	232.07	J/mol×K	504.34	Joback Method
cpg	245.84	J/mol×K	541.52	Joback Method
cpg	258.81	J/mol×K	578.69	Joback Method
cpg	271.02	J/mol×K	615.86	Joback Method
cpg	282.49	J/mol×K	653.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	1.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5597273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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