

4-Piperidinone, 2,2,6,6-tetramethyl-

Other names:	2,2,6,6-Tetramethyl-4-piperidone Triacetamin Triacetaminamine Triacetone amine Vincubina Vincubine 2,2,6,6-Tetramethyl-4-oxopiperidine 2,2,6,6-Tetramethyl-4-piperidinone 4-Piperidone, 2,2,6,6-tetramethyl- 4-Oxo-2,2,6,6-tetramethylpiperidine 2,2,6,6-Tetramethylpiperidinone 2,2,6,6-Tetramethylpiperidone Trojacetonoaminy Ikh 196 Odorotine NSC 16579 10581-38-1 (hydrate)
Inchi:	InChI=1S/C9H17NO/c1-8(2)5-7(11)6-9(3,4)10-8/h10H,5-6H2,1-4H3
InchiKey:	JWUXJYZVKZKLTJ-UHFFFAOYSA-N
Formula:	C9H17NO
SMILES:	CC1(C)CC(=O)CC(C)(C)N1
Mol. weight [g/mol]:	155.24
CAS:	826-36-8

Physical Properties

Property code	Value	Unit	Source
chs	-5636.90 ± 3.40	kJ/mol	NIST Webbook
gf	-4.22	kJ/mol	Joback Method
hf	-273.50 ± 6.20	kJ/mol	NIST Webbook
hfs	-334.30 ± 3.40	kJ/mol	NIST Webbook
hfus	8.48	kJ/mol	Joback Method
hsub	60.80 ± 2.70	kJ/mol	NIST Webbook
hvap	44.45	kJ/mol	Joback Method
ie	8.30 ± 0.05	eV	NIST Webbook
ie	7.74	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	1.496		Crippen Method

mvol	138.360	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	478.20	K	NIST Webbook
tc	778.50	K	Joback Method
tf	415.38	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.55	J/mol×K	537.05	Joback Method
cpg	355.77	J/mol×K	577.29	Joback Method
cpg	372.90	J/mol×K	617.53	Joback Method
cpg	389.13	J/mol×K	657.77	Joback Method
cpg	404.68	J/mol×K	698.01	Joback Method
cpg	419.75	J/mol×K	738.25	Joback Method
cpg	434.55	J/mol×K	778.50	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=C826368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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