2,2,6,6-Tetramethyl-4-piperidone

Other names:	10581-38-1 (hydrate) 2,2,6,6-Tetramethyl-4-oxopiperidine 2,2,6,6-Tetramethyl-4-piperidinone 2,2,6,6-Tetramethyl-4-piperidone 2,2,6,6-Tetramethylpiperidinone 2,2,6,6-Tetramethylpiperidone 4-Oxo-2,2,6,6-tetramethylpiperidine 4-Piperidone, 2,2,6,6-tetramethyl- Ikh 196 NSC 16579 Odoratine Triacetonamin Triacetonamine Triacetone amine Trojacetonoaminy Vincubina Vincubine
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

Physical Properties

Property code	Value	Unit	Source
chs	-5636.90 ± 3.40	kJ/mol	NIST Webbook
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
ie	7.74	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
logp	1.496		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
tb	478.20	K	NIST Webbook
tf	380.65	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C826368&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
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
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point