

1,2,3,6-Tetrahydropyridine

Other names:	Pyridine, 1,2,3,6-tetrahydro- «delta»3-Piperidine 1,2,5,6-Tetrahydropyridine UN 2410 Pyridine, 1,2,5,6-tetrahydro-
Inchi:	InChI=1S/C5H9N/c1-2-4-6-5-3-1/h1-2,6H,3-5H2
InchiKey:	FTAHXMZRJCZIDL-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	C1=CCNCC1
Mol. weight [g/mol]:	83.13
CAS:	694-05-3

Physical Properties

Property code	Value	Unit	Source
chl	-3287.30 ± 2.30	kJ/mol	NIST Webbook
gf	141.05	kJ/mol	Joback Method
hf	23.72	kJ/mol	Joback Method
hfl	33.00 ± 2.30	kJ/mol	NIST Webbook
hfus	10.28	kJ/mol	Joback Method
hvap	107.70	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.64 ± 0.05	eV	NIST Webbook
log10ws	-0.85		Crippen Method
logp	0.536		Crippen Method
mcvol	76.130	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
tb	381.20	K	NIST Webbook
tc	604.79	K	Joback Method
tf	263.52	K	Joback Method
vc	0.273	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	123.72	J/mol×K	385.73	Joback Method
cpg	135.93	J/mol×K	422.24	Joback Method
cpg	147.51	J/mol×K	458.75	Joback Method
cpg	158.48	J/mol×K	495.26	Joback Method
cpg	168.84	J/mol×K	531.77	Joback Method
cpg	178.61	J/mol×K	568.28	Joback Method
cpg	187.81	J/mol×K	604.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694053&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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