

3-Pyridinol, 6-methyl-

Other names:	2-Methyl-5-hydroxypyridine 3-Hydroxy-6-methylpyridine 5-Hydroxy-2-methylpyridine 6-Methyl-3-hydroxypyridine 6-Methyl-3-pyridinol 6-methylpyridin-3-ol
Inchi:	InChI=1S/C6H7NO/c1-5-2-3-6(8)4-7-5/h2-4,8H,1H3
InchiKey:	DHLUJPLHLZJUBW-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1ccc(O)cn1
Mol. weight [g/mol]:	109.13
CAS:	1121-78-4

Physical Properties

Property code	Value	Unit	Source
chs	-3195.50 ± 1.30	kJ/mol	NIST Webbook
hf	-69.80 ± 2.60	kJ/mol	NIST Webbook
hfs	-166.00 ± 1.50	kJ/mol	NIST Webbook
hsub	96.20 ± 2.10	kJ/mol	NIST Webbook
hsub	96.20 ± 2.10	kJ/mol	NIST Webbook
ie	9.15 ± 0.05	eV	NIST Webbook
log10ws	-1.26		Crippen Method
logp	1.096		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
ripol	2430.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121784&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
riol:	Polar retention indices

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