Pyridine, 3-methoxy-

Other names: «beta»-Methoxypyridine
3-Methoxypyridine
Inchi: InChI=1S/C6H7NO/c1-8-6-3-2-4-7-5-6/h2-5H,1H3
InchiKey: UMJSCPRVCHMLSP-UHFFFAOYSA-N
Formula: C6H7NO
SMILES: COc1cccnc1
Mol. weight [g/mol]: 109.13
CAS: 7295-76-3

Physical Properties

Property code	Value	Unit	Source
affp	942.70	kJ/mol	NIST Webbook
basg	910.90	kJ/mol	NIST Webbook
ie	9.34 ± 0.05	eV	NIST Webbook
ie	9.34 ± 0.02	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.090		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
rinpol	960.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	993.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1584.00		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=C7295763&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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