

Methyl picolinimide

Other names:	Methyl iminopicolinate
Inchi:	InChI=1S/C7H8N2O/c1-10-7(8)6-4-2-3-5-9-6/h2-5,8H,1H3
InchiKey:	NEGQCMNHXHSFGU-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	<chem>COC(=N)c1ccccn1</chem>
Mol. weight [g/mol]:	136.15
CAS:	19547-38-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.053		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
rinpola	1181.00		NIST Webbook
ripola	1789.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.00 ± 2.00	K	3.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C19547387&Units=SI

Legend

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
tbrp:	Boiling point at reduced pressure

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