Methyl picolinimidate

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: COC(=N)c1ccccn1
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
rinpol	1181.00		NIST Webbook
ripol	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/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=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