

1,3,4-Trimethylpyrrolo[1,2-a]pyrazine

Inchi:	InChI=1S/C10H12N2/c1-7-9(3)12-6-4-5-10(12)8(2)11-7/h4-6H,1-3H3
InchiKey:	FRLPHFSUUPGOPI-UHFFFAOYSA-N
Formula:	C10H12N2
SMILES:	Cc1nc(C)c2cccn2c1C
Mol. weight [g/mol]:	160.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.260		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
ripol	1876.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/94-339-2/1-3-4-Trimethylpyrrolo-1-2-a-pyrazine.pdf>

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