

N-(5-Methylfurfuryl)dimethylamine

Other names:	N,N,5-Trimethylfurfurylamine
Inchi:	InChI=1S/C8H13NO/c1-7-4-5-8(10-7)6-9(2)3/h4-5H,6H2,1-3H3
InchiKey:	IYULRWBZWXMBGW-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	Cc1ccc(CN(C)C)o1
Mol. weight [g/mol]:	139.19
CAS:	14496-35-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	1.650		Crippen Method
mcvol	119.970	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14496356&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

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