

2-N-nonyl-5-methyl pyrazine

Inchi:	InChI=1S/C14H24N2/c1-3-4-5-6-7-8-9-10-14-12-15-13(2)11-16-14/h11-12H,3-10H2,1-2H
InchiKey:	SUZWKGCYWNHULO-UHFFFAOYSA-N
Formula:	C14H24N2
SMILES:	CCCCCCCCc1cnc(C)cn1
Mol. weight [g/mol]:	220.35
CAS:	116660-47-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.078		Crippen Method
mcvol	204.320	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660470&Units=SI
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

Legend

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

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