

2-N-heptyl-6-methyl pyrazine

Inchi:	InChI=1S/C12H20N2/c1-3-4-5-6-7-8-12-10-13-9-11(2)14-12/h9-10H,3-8H2,1-2H3
InchiKey:	CCMUPZMBTDQOBO-UHFFFAOYSA-N
Formula:	C12H20N2
SMILES:	CCCCCCCc1cncc(C)n1
Mol. weight [g/mol]:	192.30
CAS:	32184-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.298		Crippen Method
mcvol	176.140	ml/mol	McGowan Method

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=C32184568&Units=SI

Legend

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

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