

(5-Nonyl)pyrazine

Inchi: InChI=1S/C13H22N2/c1-3-5-7-12(8-6-4-2)13-11-14-9-10-15-13/h9-12H,3-8H2,1-2H3
InchiKey: KYYGNUQVRQTODD-UHFFFAOYSA-N
Formula: C13H22N2
SMILES: CCCCC(CCCC)c1cnccn1
Mol. weight [g/mol]: 206.33
CAS: 116660-09-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.941		Crippen Method
mcvol	190.230	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660094&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

Latest version available from:

<https://www.chemeo.com/cid/83-198-1/5-Nonyl-pyrazine.pdf>

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