3,5-dimethyl-2-pentylpyrazine

Inchi: InChI=1S/C11H18N2/c1-4-5-6-7-11-10(3)13-9(2)8-12-11/h8H,4-7H2,1-3H3
InchiKey: JHECZRZZPVHFGJ-UHFFFAOYSA-N
Formula: C11H18N2
SMILES: CCCCCc1ncc(C)nc1C
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.826		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
ripol	1676.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R413328&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
ripol: Polar retention indices