2-Anilino-3-(n-pentyl) pyrazine

Inchi: InChI=1S/C15H19N3/c1-2-3-5-10-14-15(17-12-11-16-14)18-13-8-6-4-7-9-13/h4,6-9,11-12

InchiKey: BWNXCBLZSVIRSK-UHFFFAOYSA-N

Formula: C15H19N3

SMILES: CCCCCc1ncc[nH]c1=Nc1ccccc1

Mol. weight [g/mol]: 241.33

CAS: 116659-97-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.893		Crippen Method
mcvol	204.630	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=C116659973&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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