

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/h4,6-9,11-1
InchiKey:	BWNXCBLZSVIRSK-UHFFFAOYSA-N
Formula:	C15H19N3
SMILES:	CCCCCc1ncc[nH]c1=Nc1cccc1
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

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