

2-(M-bromoanilino)-3-methyl pyrazine

Inchi:	InChI=1S/C11H10BrN3/c1-8-11(14-6-5-13-8)15-10-4-2-3-9(12)7-10/h2-7H,1H3,(H,14,15)
InchiKey:	HMRYQYFCVVDVFT-UHFFFAOYSA-N
Formula:	C11H10BrN3
SMILES:	Cc1nccnc1Nc1cccc(Br)c1
Mol. weight [g/mol]:	264.12
CAS:	92847-27-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	3.291		Crippen Method
mcvol	165.770	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=C92847273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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<https://www.chemeo.com/cid/22-100-5/2-M-bromoanilino-3-methyl-pyrazine.pdf>

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