

2-Amino-3-benzyl-5-(4-methoxyphenyl)pyrazine-1-oxide

Inchi:	InChI=1S/C18H17N3O2/c1-23-15-9-7-14(8-10-15)17-12-21(22)18(19)16(20-17)11-13-5-3
InchiKey:	HWHMEJZWCZUMTH-UHFFFAOYSA-N
Formula:	C18H17N3O2
SMILES:	COc1ccc(-c2c[n+](O)c(N)c(Cc3ccccc3)n2)cc1
Mol. weight [g/mol]:	307.35
CAS:	123437-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	2.564		Crippen Method
mcvol	234.880	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123437730&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

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