

2-(2-Aminophenyl)benzimidazole

Other names:	2-(o-Aminophenyl)benzimidazole Benzenamine, 2-(1H-benzimidazol-2-yl)- 2-(1H-Benzoimidazol-2-yl)-phenylamine 2-(1H-benzimidazol-2-yl)aniline
Inchi:	InChI=1S/C13H11N3/c14-10-6-2-1-5-9(10)13-15-11-7-3-4-8-12(11)16-13/h1-8H,14H2,(H
InchiKey:	YWNXHTNWOQHFR-LUHFFFAOYSA-N
Formula:	C13H11N3
SMILES:	<chem>Nc1cccc1-c1nc2cccc2[nH]1</chem>
Mol. weight [g/mol]:	209.25
CAS:	5805-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	2.330		Crippen Method
mcvol	161.290	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5805390&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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