2(o-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:	YWNXHTNWOQHFRL-UHFFFAOYSA-N
Formula:	C13H11N3
SMILES:	Nc1ccccc1-c1nc2ccccc2[nH]1
Mol. weight [g/mol]:	209.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Cheméo Relay (1.0)
logp	2.330		Crippen Method
mcvol	161.290	ml/mol	McGowan Method
tf	521.64	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5805390&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

tf: Normal melting (fusion) point

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