

Imidazole-5(4)-sulfonanilide, 4(5)-bromo-

Inchi:	InChI=1S/C9H8BrN3O2S/c10-8-9(12-6-11-8)16(14,15)13-7-4-2-1-3-5-7/h1-6,13H,(H,11,1
InchiKey:	GPELLZGCGDMSBS-UHFFFAOYSA-N
Formula:	C9H8BrN3O2S
SMILES:	O=S(=O)(Nc1cccc1)c1[nH]cnc1Br
Mol. weight [g/mol]:	302.15
CAS:	99903-07-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	1.491		Crippen Method
mcvol	169.980	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=C99903078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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