Imidazole, 5-(o-aminophenylthio)-1-methyl-4-nitro-

Inchi:	InChI=1S/C10H10N4O2S/c1-13-6-12-9(14(15)16)10(13)17-8-5-3-2-4-7(8)11/h2-6H,11H2
InchiKey:	QYHRABNYVGQVDZ-UHFFFAOYSA-N
Formula:	C10H10N4O2S
SMILES:	Cn1cnc([N+](=O)[O-])c1Sc1ccccc1N
Mol. weight [g/mol]:	250.28
CAS:	53900-32-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	2.062		Crippen Method
mcvol	172.250	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=C53900326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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