

1-Methoxyphthalazine

Inchi:	InChI=1S/C9H8N2O/c1-12-9-8-5-3-2-4-7(8)6-10-11-9/h2-6H,1H3
InchiKey:	GESPRUVYTLDFDD-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	COc1nccc2ccccc12
Mol. weight [g/mol]:	160.17
CAS:	24953-56-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	1.638		Crippen Method
mcvol	120.280	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=C24953568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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