

1-Benzenesulfonyl-1H-pyrrole

Other names:	N-Benzenesulphonylpyrrole
Inchi:	InChI=1S/C10H9NO2S/c12-14(13,11-8-4-5-9-11)10-6-2-1-3-7-10/h1-9H
InchiKey:	PPPXRIUHKCOOMU-UHFFFAOYSA-N
Formula:	C10H9NO2S
SMILES:	O=S(=O)(c1ccccc1)n1cccc1
Mol. weight [g/mol]:	207.25
CAS:	16851-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.725		Crippen Method
mcvol	146.610	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=C16851824&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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