

2-Phenylmercapto-3-methylpyrazine

Other names:	Pyrazine, 2-methyl-3-phenylthio Pyrazine, 3-methyl-2-(phenylthio) 3-methyl-2-(phenylthio)pyrazine
Inchi:	InChI=1S/C11H10N2S/c1-9-11(13-8-7-12-9)14-10-5-3-2-4-6-10/h2-8H,1H3
InchiKey:	VTUFUZZBJQBYXKY-UHFFFAOYSA-N
Formula:	C11H10N2S
SMILES:	Cc1nccnc1Sc1cccc1
Mol. weight [g/mol]:	202.28
CAS:	91091-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	2.936		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2399.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91091020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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