

2-Benzylmercapto-3-methyl pyrazine

Inchi:	InChI=1S/C12H12N2S/c1-10-12(14-8-7-13-10)15-9-11-5-3-2-4-6-11/h2-8H,9H2,1H3
InchiKey:	YFTXLZYURWUCQR-UHFFFAOYSA-N
Formula:	C12H12N2S
SMILES:	Cc1nccnc1SCc1ccccc1
Mol. weight [g/mol]:	216.30
CAS:	74990-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.077		Crippen Method
mcvol	168.730	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74990491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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