

2-Phenyl mercapto-3-benzyl pyrazine

Inchi: InChI=1S/C17H14N2S/c1-3-7-14(8-4-1)13-16-17(19-12-11-18-16)20-15-9-5-2-6-10-15/h1-14,17-18,20-21H,15-16H2
InchiKey: WIRASIBIDHHWLP-UHFFFAOYSA-N
Formula: C17H14N2S
SMILES: c1ccc(Cc2nccnc2Sc2ccccc2)cc1
Mol. weight [g/mol]: 278.37
CAS: 116660-04-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	4.219		Crippen Method
mcvol	215.420	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660049&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

Latest version available from:

<https://www.chemeo.com/cid/17-424-2/2-Phenyl-mercapto-3-benzyl-pyrazine.pdf>

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