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