# 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
**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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**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

## Legend

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