Pyrazine, 2-pentyl-3-phenylthio

Inchi: InChI=1S/C15H18N2S/c1-2-3-5-10-14-15(17-12-11-16-14)18-13-8-6-4-7-9-13/h4,6-9,11-
InchiKey: FOIHOLTYNMLOGQ-UHFFFAOYSA-N
Formula: C15H18N2S
SMILES: CCCCCc1nccnc1Sc1ccccc1
Mol. weight [g/mol]: 258.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.361		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
ripol	2717.00		NIST Webbook
ripol	2717.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R43592&Units=SI

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