Pyrazine, 3-phenylthio-2-propyl

Other names: Pyrazine, 2-(phenylthio)-3-propyl
Inchi: InChI=1S/C13H14N2S/c1-2-6-12-13(15-10-9-14-12)16-11-7-4-3-5-8-11/h3-5,7-10H,2,6H
InchiKey: PSJZBQGNCLINMQ-UHFFFAOYSA-N
Formula: C13H14N2S
SMILES: CCCc1nccnc1Sc1ccccc1
Mol. weight [g/mol]: 230.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.580		Crippen Method
mcvol	182.820	ml/mol	McGowan Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
ripol	2532.00		NIST Webbook
ripol	2532.00		NIST Webbook

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=R43784&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
rinpol: Non-polar retention indices
ripol: Polar retention indices