Pyrazine, 2-octyl-3-phenylthio

Inchi: InChI=1S/C18H24N2S/c1-2-3-4-5-6-10-13-17-18(20-15-14-19-17)21-16-11-8-7-9-12-16/h
InchiKey: KGQCBIZAFKZZQC-UHFFFAOYSA-N
Formula: C18H24N2S
SMILES: CCCCCCCCc1nccnc1Sc1ccccc1
Mol. weight [g/mol]: 300.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	5.531		Crippen Method
mcvol	253.270	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R43574&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
rinpol: Non-polar retention indices
ripol: Polar retention indices