

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

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