

2-(P-t-butyl phenyl mercapto)-3-methylpyrazine

Inchi:	InChI=1S/C15H18N2S/c1-11-14(17-10-9-16-11)18-13-7-5-12(6-8-13)15(2,3)4/h5-10H,1-4
InchiKey:	FTLAOHYBYDZUHV-UHFFFAOYSA-N
Formula:	C15H18N2S
SMILES:	<chem>Cc1nccnc1Sc1ccc(C(C)(C)C)cc1</chem>
Mol. weight [g/mol]:	258.38
CAS:	94065-57-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.234		Crippen Method
mcvol	211.000	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=C94065573&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

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<https://www.chemeo.com/cid/85-116-9/2-P-t-butyl-phenyl-mercapto-3-methyl-pyrazine.pdf>

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