2-(P-t-butyl phenyl mercapto)-3-methyl pyrazine

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: Cc1nccnc1Sc1ccc(C(C)(C)C)cc1

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