2-(P-methoxyanilino)-3-methyl pyrazine

Inchi: InChI=1S/C12H13N3O/c1-9-12(14-8-7-13-9)15-10-3-5-11(16-2)6-4-10/h3-8H,1-2H3,(H,1
InchiKey: JZVHKOANTZWQSK-UHFFFAOYSA-N
Formula: C12H13N3O
SMILES: COc1ccc(Nc2nccnc2C)cc1
Mol. weight [g/mol]: 215.25
CAS: 88613-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.537		Crippen Method
mcvol	168.230	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88613983&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume