3-(N-methylanilino)-2,5-dimethyl pyrazine

Inchi: InChI=1S/C13H15N3/c1-10-9-14-11(2)13(15-10)16(3)12-7-5-4-6-8-12/h4-9H,1-3H3
InchiKey: XWHJNVZWHGYZGL-UHFFFAOYSA-N
Formula: C13H15N3
SMILES: Cc1cnc(C)c(N(C)c2ccccc2)n1
Mol. weight [g/mol]: 213.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	2.861		Crippen Method
mcvol	176.450	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=B6002861&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