3-Methyl-4-phenylpyrazole

Inchi: InChI=1S/C10H10N2/c1-8-10(7-11-12-8)9-5-3-2-4-6-9/h2-7H,1H3,(H,11,12)
InchiKey: XTXZCNATVCIKTR-UHFFFAOYSA-N
Formula: C10H10N2
SMILES: Cc1n[nH]cc1-c1ccccc1
Mol. weight [g/mol]: 158.20
CAS: 13788-84-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.903		Crippen Method
mcvol	128.500	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=C13788846&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