3(5)-ethyl-5(3)-phenylpyrazole

Inchi: InChI=1S/C11H12N2/c1-2-10-8-11(13-12-10)9-6-4-3-5-7-9/h3-8H,2H2,1H3,(H,12,13)
InchiKey: IENAMGDFEYXOSY-UHFFFAOYSA-N
Formula: C11H12N2
SMILES: CCc1cc(-c2ccccc2)n[nH]1
Mol. weight [g/mol]: 172.23
CAS: 141665-22-7

Physical Properties

Property code	Value	Unit	Source
affp	935.60	kJ/mol	NIST Webbook
basg	903.80	kJ/mol	NIST Webbook
log10ws	-3.86		Crippen Method
logp	2.157		Crippen Method
mcvol	142.590	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141665227&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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