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:	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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

https://www.chemeo.com/cid/78-972-7/3-5-ethyl-5-3-phenylpyrazole.pdf

Generated by Cheméo on 2024-10-12 02:21:07.296097288 +0000 UTC m=+3280529.933066536.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.