3,5-diethyl-4-methylpyrazole

Inchi: InChI=1S/C8H14N2/c1-4-7-6(3)8(5-2)10-9-7/h4-5H2,1-3H3,(H,9,10)
InchiKey: ZLCADPDOQZLZBH-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: CCc1n[nH]c(CC)c1C
Mol. weight [g/mol]: 138.21
CAS: 13618-34-3

Physical Properties

Property code	Value	Unit	Source
affp	952.80	kJ/mol	NIST Webbook
basg	919.20	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	1.361		Crippen Method
mcvol	124.080	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=C13618343&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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