

4-(Adamantan-1-yl)-1H-pyrazole

Other names: 4-(1-adamantyl)-pyrazole
Inchi: InChI=1S/C13H18N2/c1-9-2-11-3-10(1)5-13(4-9,6-11)12-7-14-15-8-12/h7-11H,1-6H2,(H,
InchiKey: KJMFWFDGPIISAX-UHFFFAOYSA-N
Formula: C13H18N2
SMILES: c1n[nH]cc1C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 202.30
CAS: 84396-62-3

Physical Properties

Property code	Value	Unit	Source
affp	913.10	kJ/mol	NIST Webbook
basg	878.90	kJ/mol	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.396		Crippen Method
mcvol	161.950	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=C84396623&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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