

1-(Adamantan-1-yl)pyrazole

Other names:	1-(1-adamantyl)pyrazole
Inchi:	InChI=1S/C13H18N2/c1-2-14-15(3-1)13-7-10-4-11(8-13)6-12(5-10)9-13/h1-3,10-12H,4-9
InchiKey:	TWAYEKHIDSYYHV-UHFFFAOYSA-N
Formula:	C13H18N2
SMILES:	<chem>c1cnn(C23CC4CC(CC(C4)C2)C3)c1</chem>
Mol. weight [g/mol]:	202.30
CAS:	92234-54-3

Physical Properties

Property code	Value	Unit	Source
affp	954.50	kJ/mol	NIST Webbook
basg	922.40	kJ/mol	NIST Webbook
log10ws	-3.48		Crippen Method
logp	2.808		Crippen Method
mcvol	161.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92234543&Units=SI
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

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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<https://www.chemeo.com/cid/24-337-1/1-Adamantan-1-yl-pyrazole.pdf>

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