

Indeno[1,2-c]pyrazol-4-one, 7-chloro-3-propyl-, hydrazone

Inchi:	InChI=1S/C13H13ClN4/c1-2-3-10-11-12(16-15)8-5-4-7(14)6-9(8)13(11)18-17-10/h4-6H,2
InchiKey:	XRDHJIPTZQXACU-FOWTUZBSSA-N
Formula:	C13H13ClN4
SMILES:	CCCc1n[nH]c2c1C(=NN)c1ccc(Cl)cc1-2
Mol. weight [g/mol]:	260.72
CAS:	116434-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	2.225		Crippen Method
mcvol	187.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116434721&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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