Norharmane, N-acetyl-

Inchi: InChI=1S/C13H10N2O/c1-9(16)15-12-5-3-2-4-10(12)11-6-7-14-8-13(11)15/h2-8H,1H3
InchiKey: GDEFUERKFIJYRD-UHFFFAOYSA-N
Formula: C13H10N2O
SMILES: CC(=O)n1c2ccccc2c2ccncc21
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	2.850		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook

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=U374783&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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