

2-Phenacyl-quinoxaline

Other names:	Ethanone, 1-phenyl-2-(2-quinoxaliny)-
Inchi:	InChI=1S/C16H12N2O/c19-16(12-6-2-1-3-7-12)10-13-11-17-14-8-4-5-9-15(14)18-13/h1-5
InchiKey:	SVDCSMOJGNIGMS-UHFFFAOYSA-N
Formula:	C16H12N2O
SMILES:	O=C(Cc1cnc2ccccc2n1)c1ccccc1
Mol. weight [g/mol]:	248.28
CAS:	16310-38-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	3.055		Crippen Method
mcvol	190.850	ml/mol	McGowan Method

Sources

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=C16310386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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