Pyroquilon

Other names:	1,2,5,6-Tetrahydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one
	4H-Pyrrolo[3,2,1-ij]quinolin-4-one, 1,2,5,6-tetrahydro-
Inchi:	InChI=1S/C11H11NO/c13-10-5-4-8-2-1-3-9-6-7-12(10)11(8)9/h1-3H,4-7H2
InchiKey:	XRJLAOUDSILTFT-UHFFFAOYSA-N
Formula:	C11H11NO
SMILES:	O=C1CCc2cccc3c2N1CC3
Mol. weight [g/mol]:	173.21
CAS:	57369-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.522		Crippen Method
mcvol	131.920	ml/mol	McGowan Method
rinpol	1837.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1837.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57369321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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