

2-Methyl-4-oxo-1,4a,9-triazafluorene

Inchi:	InChI=1S/C11H9N3O/c1-7-6-10(15)14-9-5-3-2-4-8(9)13-11(14)12-7/h2-6H,1H3,(H,12,13)
InchiKey:	GGBPUPFQFFGKLR-UHFFFAOYSA-N
Formula:	C11H9N3O
SMILES:	Cc1cc(=O)n2c(n1)[nH]c1cccc12
Mol. weight [g/mol]:	199.21
CAS:	50290-51-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	1.002		Crippen Method
mcvol	143.280	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=C50290512&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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