

7-methyl-4-azafluorenone

Inchi:	InChI=1S/C13H9NO/c1-8-4-5-9-11(7-8)13(15)10-3-2-6-14-12(9)10/h2-7H,1H3
InchiKey:	VLDRRMZGWBOCNV-UHFFFAOYSA-N
Formula:	C13H9NO
SMILES:	<chem>Cc1ccc2c(c1)C(=O)c1cccnc1-2</chem>
Mol. weight [g/mol]:	195.22
CAS:	64292-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	2.601		Crippen Method
mcvol	147.200	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=C64292020&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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