

6(5H)-Phenanthridinone

Other names:	6-Phenanthridinol 6-Phenanthridone 6(5H)-Phenanthridinone Phenanthridone Phenanthridone phenanthridin-6(5H)-one
Inchi:	InChI=1S/C13H9NO/c15-13-11-7-2-1-5-9(11)10-6-3-4-8-12(10)14-13/h1-8H,(H,14,15)
InchiKey:	RZFVLEJOHSLEFR-UHFFFAOYSA-N
Formula:	C13H9NO
SMILES:	O=c1[nH]c2ccccc2c2ccccc12
Mol. weight [g/mol]:	195.22
CAS:	1015-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.199		Crippen Method
mcvol	147.200	ml/mol	McGowan Method
tf	564.65 ± 2.00	K	NIST Webbook
tf	565.15 ± 2.00	K	NIST Webbook

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=C1015890&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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