Acenaphtho(1,2-b)pyridine

Other names:	7-Azafluoranthene
	Acenaphtho[1.2-b]pyridine
Inchi:	InChI=1S/C15H9N/c1-4-10-5-2-7-13-14(10)11(6-1)12-8-3-9-16-15(12)13/h1-9H
InchiKey:	XJWJTIKXJYAHBE-UHFFFAOYSA-N
Formula:	C15H9N
SMILES:	c1cnc2c(c1)-c1cccc3cccc-2c13
Mol. weight [g/mol]:	203.24
CAS:	206-49-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	3.882		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
rinpol	350.37		NIST Webbook
rinpol	351.38		NIST Webbook
rinpol	350.50		NIST Webbook
tb	670.00	K	NIST Webbook
tf	369.50 ± 0.50	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C206495&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point