Naphtho(2,1-f)quinoline

Other names:	1-Azachrysene
	Naphtho[2.1-f]quinoline
Inchi:	InChI=1S/C17H11N/c1-2-5-13-12(4-1)7-8-15-14(13)9-10-17-16(15)6-3-11-18-17/h1-11H
InchiKey:	ZKWHSGRDDNYNAN-UHFFFAOYSA-N
Formula:	C17H11N
SMILES:	c1ccc2c(c1)ccc1c3cccnc3ccc21
Mol. weight [g/mol]:	229.28
CAS:	218-08-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	4.541		Crippen Method
mcvol	178.230	ml/mol	McGowan Method
rinpol	407.18		NIST Webbook
rinpol	407.18		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C218086&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