Naphtho(2,1,8-def)quinoline

Other names: 1-Azapyrene
Inchi: InChI=1S/C15H9N/c1-2-10-4-5-12-8-9-16-13-7-6-11(3-1)14(10)15(12)13/h1-9H
InchiKey: QHADMMAFBAZFTE-UHFFFAOYSA-N
Formula: C15H9N
SMILES: c1cc2ccc3ccnc4ccc(c1)c2c34
Mol. weight [g/mol]: 203.24
CAS: 313-80-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	3.979		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
rinpol	358.18		NIST Webbook
rinpol	357.73		NIST Webbook
rinpol	357.73		NIST Webbook
rinpol	358.18		NIST Webbook

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=C313804&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices