

Naphtho[1,8',8:c,d]cycloundeca-1,5-diyne

Inchi:	InChI=1S/C18H14/c1-2-4-6-10-16-12-8-14-17-13-7-11-15(18(16)17)9-5-3-1/h7-8,11-14H
InchiKey:	GKARVRHBRAROLL-UHFFFAOYSA-N
Formula:	C18H14
SMILES:	C1#Cc2cccc3cccc(c23)C#CCCCC1
Mol. weight [g/mol]:	230.30
CAS:	32137-39-6

Physical Properties

Property code	Value	Unit	Source
ie	7.50	eV	NIST Webbook
log10ws	-6.24		Crippen Method
logp	4.117		Crippen Method
mcvol	193.200	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32137396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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