

Naphtho[1,8',8:c,d]cyclododeca-1,6-diyne

Inchi:	InChI=1S/C19H16/c1-2-4-6-10-16-12-8-14-18-15-9-13-17(19(16)18)11-7-5-3-1/h8-9,12-1
InchiKey:	KMTZDSUZEKFULR-UHFFFAOYSA-N
Formula:	C19H16
SMILES:	C1#Cc2cccc3cccc(c23)C#CCCCC1
Mol. weight [g/mol]:	244.33
CAS:	87842-94-2

Physical Properties

Property code	Value	Unit	Source
ie	7.48	eV	NIST Webbook
log10ws	-6.66		Crippen Method
logp	4.507		Crippen Method
mcvol	207.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87842942&Units=SI
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

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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