

Naphtho[1,8',8:c,d]cyclodeca-1,5-diiyne

Inchi: InChI=1S/C17H12/c1-2-4-8-14-10-6-12-16-13-7-11-15(17(14)16)9-5-3-1/h6-7,10-13H,1-3
InchiKey: BCDQQLPFQVULRT-UHFFFAOYSA-N
Formula: C17H12
SMILES: C1#Cc2cccc3cccc(c23)C#CCCC1
Mol. weight [g/mol]: 216.28
CAS: 32137-40-9

Physical Properties

Property code	Value	Unit	Source
ie	7.53	eV	NIST Webbook
log10ws	-5.83		Crippen Method
logp	3.727		Crippen Method
mcvol	179.110	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C32137409&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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