

2H-Cyclopenta[I]phenanthrene

Inchi:	InChI=1S/C17H12/c1-3-8-14-12(6-1)13-7-2-4-9-15(13)17-11-5-10-16(14)17/h1-4,6-11H,5
InchiKey:	BZFTXMNGGSHPN-UHFFFAOYSA-N
Formula:	C17H12
SMILES:	<chem>C1=c2c(c3ccccc3c3ccccc23)=CC1</chem>
Mol. weight [g/mol]:	216.28
CAS:	235-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	2.958		Crippen Method
mcvol	172.550	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=C235916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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