

2H-Benzo[cd]pyrene

Inchi:	InChI=1S/C19H12/c1-3-12-7-9-14-10-8-13-4-2-6-16-11-15(5-1)17(12)19(14)18(13)16/h1-
InchiKey:	QFPJPOONTXRLHG-UHFFFAOYSA-N
Formula:	C19H12
SMILES:	C1=c2ccc3cccc4cc5cccc(c5c2c34)C1
Mol. weight [g/mol]:	240.30
CAS:	191-32-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	4.202		Crippen Method
mvol	185.570	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=C191322&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
mvol:	McGowan's characteristic volume

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