

Benzo[de]cyclopent[a]anthracene

Inchi:	InChI=1S/C20H12/c1-2-8-16-14(5-1)12-19-17-9-3-6-13(17)11-15-7-4-10-18(16)20(15)19
InchiKey:	FZPMEKAWJMWZAT-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	C1=Cc2cc3ccccc4c5ccccc5cc(c2=C1)c34
Mol. weight [g/mol]:	252.31
CAS:	198-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	4.672		Crippen Method
mcvol	195.360	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=C198469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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