

Benzo[fg]cyclopent[a]anthracene

Inchi:	InChI=1S/C20H12/c1-5-14-6-3-9-18-17-11-10-13-4-2-8-16(13)19(17)12-15(7-1)20(14)18
InchiKey:	UWTVIOBLCIMLGH-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	C1=Cc2ccc3c(cc4cccc5cccc3c54)c2=C1
Mol. weight [g/mol]:	252.31
CAS:	200-63-5

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=C200635&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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