

Benzo[de]cyclopent[b]anthracene

Inchi:	InChI=1S/C20H12/c1-2-7-16-13(5-1)11-15-12-14-6-3-8-17(14)19-10-4-9-18(16)20(15)19
InchiKey:	YSQZAGVZEGZLSD-UHFFFAOYSA-N
Formula:	C20H12
SMILES:	C1=Cc2cc3cc4ccccc4c4cccc(c2=C1)c34
Mol. weight [g/mol]:	252.31
CAS:	27706-08-7

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27706087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/72-757-2/Benzo-de-cyclopent-b-anthracene.pdf>

Generated by Cheméo on 2024-05-02 20:08:22.873285145 +0000 UTC m=+16969751.793862456.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.