

Dibenzo(b,def)carbazole

Inchi: InChI=1S/C18H11N/c1-2-6-13-12(4-1)10-16-18-14(13)9-8-11-5-3-7-15(19-16)17(11)18/h
InchiKey: MOBQGBVFDKCBQD-UHFFFAOYSA-N
Formula: C18H11N
SMILES: c1ccc2c(c1)cc1[nH]c3cccc4ccc2c1c43
Mol. weight [g/mol]: 241.29
CAS: 104313-09-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	4.583		Crippen Method
mcvol	181.460	ml/mol	McGowan Method
rinpol	458.20		NIST Webbook
rinpol	458.20		NIST Webbook
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook

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=C104313099&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/78-250-8/Dibenzo-b-def-carbazole.pdf>

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