

Benz[mno]aceanthrylene

Inchi:	InChI=1S/C18H10/c1-3-11-7-8-15-10-14-6-2-5-13-9-12(4-1)16(11)18(15)17(13)14/h1-10
InchiKey:	VTNIIXMYGKMYOT-UHFFFAOYSA-N
Formula:	C18H10
SMILES:	C1=c2ccc3cccc4cc5cccc1c5c2c34
Mol. weight [g/mol]:	226.27
CAS:	203-13-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	4.007		Crippen Method
mcvol	171.480	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=C203134&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

Latest version available from:

<https://www.chemeo.com/cid/73-778-8/Benz-mno-aceanthrylene.pdf>

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