

cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, butylboronate

InChI: InChI=1S/C19H21BO2/c1-3-4-13-20-21-18-16-11-6-5-9-14(16)15-10-7-8-12-17(15)19(18)
InChIKey: NTXPIWNBXRJXPFP-MOPGFXCFSAN

Formula: C19H21BO2
SMILES: CCCCB1OC2c3ccccc3-c3ccccc3C2(C)O1
Mol. weight [g/mol]: 292.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	4.959		Crippen Method
rinpol	2125.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109574&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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