

cis-Anthracene, 1,2,3,4-tetrahydro-1,2-diol, butylboronate

Inchi: InChI=1S/C18H21BO2/c1-2-3-10-19-20-17-9-8-15-11-13-6-4-5-7-14(13)12-16(15)18(17)
InchiKey: YPPBZYZWJBTQAO-MSOLQXFVSA-N
Formula: C18H21BO2
SMILES: CCCCCB1OC2CCc3cc4ccccc4cc3C2O1
Mol. weight [g/mol]: 280.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	4.531		Crippen Method
rinpol	2235.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109321&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-579-5/cis-Anthracene-1-2-3-4-tetrahydro-1-2-diol-butylboronate.pdf>

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