

cis-Acenaphthen-1,2-diol, butylboronate

Inchi: InChI=1S/C16H17BO2/c1-2-3-10-17-18-15-12-8-4-6-11-7-5-9-13(14(11)12)16(15)19-17/H
InchiKey: VCNRMTRRMLFHEA-IYBDPMPFKSA-N
Formula: C16H17BO2
SMILES: CCCC(B1OC2c3cccc4cccc(c34)C2O1
Mol. weight [g/mol]: 252.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	4.271		Crippen Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109272&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/68-798-2/cis-Acenaphthen-1-2-diol-butylboronate.pdf>

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