

2,4-Dichlorobenzeneboronate, guaifenesin

Inchi: InChI=1S/C16H15BCl2O4/c1-20-15-4-2-3-5-16(15)21-9-12-10-22-17(23-12)13-7-6-11(18)
InchiKey: UOKGSFKRNDHNDP-UHFFFAOYSA-N
Formula: C16H15BCl2O4
SMILES: COc1ccccc1OCC1COB(c2ccc(Cl)cc2Cl)O1
Mol. weight [g/mol]: 353.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	3.192		Crippen Method
rinpol	2489.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R146697&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/44-270-3/2-4-Dichlorobenzeneboronate-guaifenesin.pdf>

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