

brodimoprim

Inchi:	InChI=1S/C13H15BrN4O2/c1-19-9-4-7(5-10(20-2)11(9)14)3-8-6-17-13(16)18-12(8)15/h4
InchiKey:	BFCRRLMMHNLSCP-UHFFFAOYSA-N
Formula:	C13H15Cl2N3
SMILES:	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1Br
Mol. weight [g/mol]:	284.18
CAS:	56518-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.011		Crippen Method
mcpvol	215.670	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	49.90	kJ/mol	505.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56518413&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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