

Purine, 6-amino-8-bromo, TMS

Inchi: InChI=1S/C8H12BrN5Si/c1-15(2,3)14-7-5-6(10-4-11-7)13-8(9)12-5/h4H,1-3H3,(H2,10,11)
InchiKey: RJUHXTFCGGMIW-UHFFFAOYSA-N
Formula: C8H12BrN5Si
SMILES: C[Si](C)(C)Nc1ncnc2nc(Br)[nH]c12
Mol. weight [g/mol]: 286.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	1.880		Crippen Method
rinpol	2053.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386553&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/48-062-0/Purine-6-amino-8-bromo-TMS.pdf>

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