Pyrimidine, 6-amino-2,4-dichloro-5-nitro, TMS

Inchi: InChI=1S/C7H10Cl2N4O2Si/c1-16(2,3)12-6-4(13(14)15)5(8)10-7(9)11-6/h1-3H3,(H,10,11

InchiKey: XBEIZFSSOAPXBA-UHFFFAOYSA-N

Formula: C7H10Cl2N4O2Si

SMILES: C[Si](C)(C)Nc1nc(Cl)nc(Cl)c1[N+](=O)[O-]

Mol. weight [g/mol]: 281.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	2.938		Crippen Method
rinpol	1961.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R387036&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/10-064-9/Pyrimidine-6-amino-2-4-dichloro-5-nitro-TMS.pdf
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