

5-Mercaptouracil, TMS

Inchi: InChI=1S/C13H28N2O2SSi3/c1-19(2,3)16-12-11(18-21(7,8)9)10-14-13(15-12)17-20(4,5)
InchiKey: WWFXIHDKLJGBKU-UHFFFAOYSA-N
Formula: C13H28N2O2SSi3
SMILES: C[Si](C)(C)Oc1ncc(S[Si](C)(C)C)c(O[Si](C)(C)C)n1
Mol. weight [g/mol]: 360.69

Physical Properties

Property code	Value	Unit	Source
log10ws	1.35		Crippen Method
logp	4.831		Crippen Method
rinsol	1729.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R93878&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/112-976-4/5-Mercaptouracil-TMS.pdf>

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