4-Neopentyloxypyrimidine-2-thiol

Inchi: InChI=1S/C9H14N2OS/c1-9(2,3)6-12-7-4-5-10-8(13)11-7/h4-5H,6H2,1-3H3,(H,10,11,13)
InchiKey: FNQDJRJQSXMOND-UHFFFAOYSA-N
Formula: C9H14N2OS
SMILES: CC(C)(C)COc1ccnc(S)n1
Mol. weight [g/mol]: 198.28
CAS: 119612-61-2

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.190		Crippen Method
mcvol	156.090	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C119612612&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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