

3-(1'-Hydroxy-2'-pentyl) mercaptothiophene

Inchi:	InChI=1S/C9H14OS2/c1-2-3-8(6-10)12-9-4-5-11-7-9/h4-5,7-8,10H,2-3,6H2,1H3
InchiKey:	BZZVHVLJDIGMDJ-UHFFFAOYSA-N
Formula:	C9H14OS2
SMILES:	CCCC(CO)Sc1ccsc1
Mol. weight [g/mol]:	202.34
CAS:	116529-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	3.001		Crippen Method
mcvol	156.780	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=C116529125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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