

# Iso-octyl[2-(3-methylpyrazyl)] mercapto acetate

<b>Inchi:</b>	InChI=1S/C15H24N2O2S/c1-12(2)7-5-4-6-10-19-14(18)11-20-15-13(3)16-8-9-17-15/h8-9
<b>InchiKey:</b>	VIEVDFPVUOANRV-UHFFFAOYSA-N
<b>Formula:</b>	C15H24N2O2S
<b>SMILES:</b>	Cc1nccnc1SCC(=O)OCCCCC(C)C
<b>Mol. weight [g/mol]:</b>	296.43
<b>CAS:</b>	131346-17-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	3.637		Crippen Method
mcvol	242.200	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C131346173&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C131346173&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/15-010-3/Iso-octyl-2-3-methylpyrazyl-mercapto-acetate.pdf>

Generated by Cheméo on 2024-04-30 03:25:04.697663877 +0000 UTC m=+16736753.618241188.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.