

2-(T-nonylmercapto)-3-methyl pyrazine

Inchi:	InChI=1S/C14H24N2S/c1-5-6-7-8-9-14(3,4)17-13-12(2)15-10-11-16-13/h10-11H,5-9H2,1
InchiKey:	JWEABFCWMGFYBA-UHFFFAOYSA-N
Formula:	C14H24N2S
SMILES:	CCCCCCC(C)(C)Sc1nccnc1C
Mol. weight [g/mol]:	252.42
CAS:	2850-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	4.626		Crippen Method
mcvol	220.670	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2850773&Units=SI

Legend

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

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<https://www.chemeo.com/cid/118-480-8/2-T-nonylmercapto-3-methyl-pyrazine.pdf>

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