

# Pyrazine, 3-ethylthio-2-pentyl

<b>Other names:</b>	Pyrazine, 2-(ethylthio)-3-pentyl
<b>Inchi:</b>	InChI=1S/C11H18N2S/c1-3-5-6-7-10-11(14-4-2)13-9-8-12-10/h8-9H,3-7H2,1-2H3
<b>InchiKey:</b>	MBFGUEWRWPOKQU-UHFFFAOYSA-N
<b>Formula:</b>	C11H18N2S
<b>SMILES:</b>	CCCCCc1nccnc1SCC
<b>Mol. weight [g/mol]:</b>	210.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	3.321		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpol	1576.00		NIST Webbook
ripol	1995.00		NIST Webbook

## 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=R43695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R43695&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/69-538-9/Pyrazine-3-ethylthio-2-pentyl.pdf>

Generated by Cheméo on 2024-04-26 07:34:05.148627111 +0000 UTC m=+16406094.069204424.

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