Pyrazine, 3-ethylthio-2-pentyl

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

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=R43695&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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