2-ethylthio-3-methyl-5-(2-methylpentyl)pyrazine

Inchi: InChI=1S/C13H22N2S/c1-5-7-10(3)8-12-9-14-13(16-6-2)11(4)15-12/h9-10H,5-8H2,1-4H3
InchiKey: JLGYHZWFTNTWFR-UHFFFAOYSA-N
Formula: C13H22N2S
SMILES: CCCC(C)Cc1cnc(SCC)c(C)n1
Mol. weight [g/mol]: 238.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	3.876		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	1686.00		NIST Webbook
ripol	2026.00		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=R38377&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