

Pyrazine, 2-decyl-3-ethylthio

Inchi: InChI=1S/C16H28N2S/c1-3-5-6-7-8-9-10-11-12-15-16(19-4-2)18-14-13-17-15/h13-14H,3
InchiKey: TWSNPHWLYURUAE-UHFFFAOYSA-N
Formula: C16H28N2S
SMILES: CCCCCCCCCc1nccnc1SCC
Mol. weight [g/mol]: 280.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.272		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
ripol	2520.00		NIST Webbook
ripol	2520.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R43403&Units=SI>

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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