

2-Thiopheneacetamide, N-(2-ethylhexyl)-

Inchi: InChI=1S/C14H23NOS/c1-3-5-7-12(4-2)11-15-14(16)10-13-8-6-9-17-13/h6,8-9,12H,3-5,7
InchiKey: NFHCBWIMPRHLFX-UHFFFAOYSA-N
Formula: C14H23NOS
SMILES: CCCCC(CC)CNC(=O)Cc1cccs1
Mol. weight [g/mol]: 253.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	3.623		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinsol	2014.00		NIST Webbook
rinsol	2014.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407011&Units=SI>
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>

Legend

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

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