

2-Thiopheneacetamide, N,N-diheptyl-

Inchi: InChI=1S/C20H35NOS/c1-3-5-7-9-11-15-21(16-12-10-8-6-4-2)20(22)18-19-14-13-17-23-
InchiKey: IPQJRPQIIIJTIX-UHFFFAOYSA-N
Formula: C20H35NOS
SMILES: CCCCCCN(CCCCCC)C(=O)Cc1cccs1
Mol. weight [g/mol]: 337.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	6.060		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
rinsol	2491.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308140&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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