

2-Thiopheneacetamide, N-hexadecyl-

Inchi: InChI=1S/C22H39NOS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-23-22(24)20-21-17-16-
InchiKey: XJIPCLVNCYLICS-UHFFFAOYSA-N
Formula: C22H39NOS
SMILES: CCCCCCCCCCCCCCN=C(O)Cc1cccs1
Mol. weight [g/mol]: 365.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.71		Crippen Method
logp	7.728		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
rinsol	2980.00		NIST Webbook
rinsol	2980.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407019&Units=SI>

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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