2-Thiopheneacetamide, N-octyl-

Inchi: InChI=1S/C14H23NOS/c1-2-3-4-5-6-7-10-15-14(16)12-13-9-8-11-17-13/h8-9,11H,2-7,10
InchiKey: ANYASKWXRIUZJK-UHFFFAOYSA-N
Formula: C14H23NOS
SMILES: CCCCCCCCNC(=O)Cc1cccs1
Mol. weight [g/mol]: 253.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.767		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407013&Units=SI
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

Legend

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

Latest version available from:
https://www.chemeo.com/cid/122-255-3/2-Thiopheneacetamide-N-octyl.pdf
Generated by Cheméo on 2024-05-03 04:41:11.739310738 +0000 UTC m=+17000520.659888050.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.