2-Thiopheneacetamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C21H37NOS/c1-3-5-7-9-11-13-17-22(16-12-10-8-6-4-2)21(23)19-20-15-14-18-
InchiKey: AHJWTKRJFXGBHN-UHFFFAOYSA-N
Formula: C21H37NOS
SMILES: CCCCCCCCN(CCCCCCC)C(=O)Cc1cccs1
Mol. weight [g/mol]: 351.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.66		Crippen Method
logp	6.450		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308141&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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