2-Thiophenecarboxamide, N-(hept-2-yl)-

Inchi: InChI=1S/C12H19NOS/c1-3-4-5-7-10(2)13-12(14)11-8-6-9-15-11/h6,8-10H,3-5,7H2,1-2H
InchiKey: FCLHURNQXYAFJF-UHFFFAOYSA-N
Formula: C12H19NOS
SMILES: CCCCCC(C)NC(=O)c1cccs1
Mol. weight [g/mol]: 225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.447		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpol	1857.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407026&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