Furan-2-carboxamide, N-heptyl-n-octyl-

Inchi: InChI=1S/C20H35NO2/c1-3-5-7-9-11-13-17-21(16-12-10-8-6-4-2)20(22)19-15-14-18-23-
InchiKey: ALZKYQSUFTXZLX-UHFFFAOYSA-N
Formula: C20H35NO2
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccco1
Mol. weight [g/mol]: 321.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.79		Crippen Method
logp	6.053		Crippen Method
mcvol	290.620	ml/mol	McGowan Method
rinpol	2323.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U308208&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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