Propanamide, 3-phenyl-N-dodecyl-

Inchi: InChI=1S/C21H35NO/c1-2-3-4-5-6-7-8-9-10-14-19-22-21(23)18-17-20-15-12-11-13-16-2(
InchiKey: VEFOCGBVOIIWQQ-UHFFFAOYSA-N
Formula: C21H35NO
SMILES: CCCCCCCCCCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
hf	-320.04	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.497		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
tb	875.30	K	Joback Method
tc	1075.76	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407159&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature