

Propanamide, 3-phenyl-N-hexadecyl-

Inchi: InChI=1S/C25H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-23-26-25(27)22-21-24-19-1
InchiKey: KRGZTACOEPAZLB-UHFFFAOYSA-N
Formula: C25H43NO
SMILES: CCCCCCCCCCCCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 373.62

Physical Properties

Property code	Value	Unit	Source
hf	-402.60	kJ/mol	Joback Method
hvap	93.59	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.057		Crippen Method
mcvol	350.900	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	3114.00		NIST Webbook
tb	966.82	K	Joback Method
tc	1184.21	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407161&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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