Propanamide, 3-phenyl-N-octadecyl-

Inchi: InChI=1S/C27H47NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-25-28-27(29)24-23-2
InchiKey: OGEPYHVHEMOTBL-UHFFFAOYSA-N
Formula: C27H47NO
SMILES: CCCCCCCCCCCCCCCCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
hf	-443.88	kJ/mol	Joback Method
hvap	98.04	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.837		Crippen Method
mcvol	379.080	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
rinpol	3347.00		NIST Webbook
rinpol	3347.00		NIST Webbook
tb	1012.58	K	Joback Method
tc	1244.69	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407162&Units=SI
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

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