

Propanamide, 3-cyclopentyl-N-tetradecyl

Inchi: InChI=1S/C22H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-15-20-23-22(24)19-18-21-16-13-14-1
InchiKey: SVNCCAAKTZTAKY-UHFFFAOYSA-N
Formula: C22H43NO
SMILES: CCCCCCCCCCCCCCN=C(O)CCC1CCCC1
Mol. weight [g/mol]: 337.58

Physical Properties

Property code	Value	Unit	Source
hf	-516.73	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	7.614		Crippen Method
mcvol	321.530	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook
tb	886.78	K	Joback Method
tc	1086.28	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407387&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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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