

Propanamide, 3-cyclopentyl-N-octyl-

Inchi:	InChI=1S/C16H31NO/c1-2-3-4-5-6-9-14-17-16(18)13-12-15-10-7-8-11-15/h15H,2-14H2,
InchiKey:	ZFVNUJJUYXHVNH-UHFFFAOYSA-N
Formula:	C16H31NO
SMILES:	CCCCCCCCN=C(O)CCC1CCCC1
Mol. weight [g/mol]:	253.42

Physical Properties

Property code	Value	Unit	Source
hf	-392.89	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	5.274		Crippen Method
mcvol	236.990	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	749.50	K	Joback Method
tc	938.48	K	Joback Method

Sources

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=U407382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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