

Propanamide, 3-cyclopentyl-N-(hept-2-yl)-

Inchi:	InChI=1S/C15H29NO/c1-3-4-5-8-13(2)16-15(17)12-11-14-9-6-7-10-14/h13-14H,3-12H2,1
InchiKey:	JXODAYBHLJGKHW-UHFFFAOYSA-N
Formula:	C15H29NO
SMILES:	CCCCC(C)N=C(O)CCC1CCCC1
Mol. weight [g/mol]:	239.40

Physical Properties

Property code	Value	Unit	Source
hf	-377.53	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.882		Crippen Method
mcvol	222.900	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	726.18	K	Joback Method
tc	918.19	K	Joback Method

Sources

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=U407379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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