Carbonic acid, monoamide, N-hexyl-, octyl ester

Inchi: InChI=1S/C15H31NO2/c1-3-5-7-9-10-12-14-18-15(17)16-13-11-8-6-4-2/h3-14H2,1-2H3,(

InchiKey: RURCHJQJCVWZIA-UHFFFAOYSA-N

Formula: C15H31NO2

SMILES: CCCCCCCCOC(O)=NCCCCCC

Mol. weight [g/mol]: 257.41

Physical Properties

Property code	Value	Unit	Source
hf	-564.95	kJ/mol	Joback Method
hvap	71.47	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.858		Crippen Method
mcvol	239.630	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	733.76	K	Joback Method
tc	909.33	K	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U406457&Units=SI

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