Carbonic acid, monoamide, N-heptyl-, but-3-yn-1-yl ester

Inchi: InChI=1S/C12H21NO2/c1-3-5-7-8-9-10-13-12(14)15-11-6-4-2/h2H,3,5-11H2,1H3,(H,13,1

InchiKey: PDKJSRWSPUITJD-UHFFFAOYSA-N

Formula: C12H21NO2

SMILES: C#CCCOC(O)=NCCCCCCC

Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
hf	-211.13	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.911		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	655.24	K	Joback Method
tc	837.04	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=U415465&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