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

Inchi: InChI=1S/C19H35NO2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-20-19(21)22-18-6-4-2/h2H

InchiKey: VSVUELBYPBHVOE-UHFFFAOYSA-N

Formula: C19H35NO2

SMILES: C#CCCOC(O)=NCCCCCCCCCCCCCC

Mol. weight [g/mol]: 309.49

Physical Properties

Property code	Value	Unit	Source
hf	-355.61	kJ/mol	Joback Method
hvap	80.23	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.641		Crippen Method
mcvol	287.390	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2741.00		NIST Webbook
tb	815.40	K	Joback Method
tc	1001.61	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415471&Units=SI

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

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