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

Inchi: InChI=1S/C23H43NO2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-23(25)26-

InchiKey: XMCJICCUXMSKAG-UHFFFAOYSA-N

Formula: C23H43NO2

SMILES: C#CCCOC(O)=NCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 365.59

Physical Properties

Property code	Value	Unit	Source
hf	-438.17	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.202		Crippen Method
mcvol	343.750	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	906.92	K	Joback Method
tc	1111.08	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415473&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

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

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