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

Inchi: InChI=1S/C21H39NO2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-22-21(23)24-20-6-4

InchiKey: KQMVFUAMARSWQX-UHFFFAOYSA-N

Formula: C21H39NO2

SMILES: C#CCCOC(O)=NCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 337.54

Physical Properties

Property code	Value	Unit	Source
hf	-396.89	kJ/mol	Joback Method
hvap	84.68	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.422		Crippen Method
mcvol	315.570	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	861.16	K	Joback Method
tc	1054.57	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415472&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