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

Inchi: InChI=1S/C14H25NO2/c1-3-5-7-8-9-10-11-12-15-14(16)17-13-6-4-2/h2H,3,5-13H2,1H3,(

InchiKey: LVRIQCSNIVHDBP-UHFFFAOYSA-N

Formula: C14H25NO2

SMILES: C#CCCOC(=O)NCCCCCCCCC

Mol. weight [g/mol]: 239.35

Physical Properties

Property code	Value	Unit	Source
gf	145.54	kJ/mol	Joback Method
hf	-231.72	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.486		Crippen Method
mcvol	216.940	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
tb	636.30	K	Joback Method
tc	815.19	K	Joback Method
tf	419.33	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.80	J/mol×K	636.30	Joback Method
cpg	597.55	J/mol×K	666.12	Joback Method
cpg	612.57	J/mol×K	695.93	Joback Method
cpg	626.87	J/mol×K	725.75	Joback Method
cpg	640.48	J/mol×K	755.56	Joback Method
cpg	653.41	J/mol×K	785.38	Joback Method
cpg	665.69	J/mol×K	815.19	Joback Method

Sources

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=U415467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume