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

Inchi: InChI=1S/C16H29NO2/c1-3-5-7-8-9-10-11-12-13-14-17-16(18)19-15-6-4-2/h2H,3,5-15H2

InchiKey: ZHRDNAAQVZEPNF-UHFFFAOYSA-N

Formula: C16H29NO2

SMILES: C#CCCOC(=O)NCCCCCCCCCCC

Mol. weight [g/mol]: 267.41

Physical Properties

Property code	Value	Unit	Source
gf	162.38	kJ/mol	Joback Method
hf	-273.00	kJ/mol	Joback Method
hfus	48.06	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.267		Crippen Method
mcvol	245.120	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	682.06	K	Joback Method
tc	859.54	K	Joback Method
tf	441.87	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.38	J/mol×K	682.06	Joback Method
cpg	707.06	J/mol×K	711.64	Joback Method
cpg	722.95	J/mol×K	741.22	Joback Method
cpg	738.06	J/mol×K	770.80	Joback Method
cpg	752.43	J/mol×K	800.38	Joback Method
cpg	766.07	J/mol×K	829.96	Joback Method
cpg	779.00	J/mol×K	859.54	Joback Method

Sources

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=U415469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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