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

Inchi: InChI=1S/C17H31NO2/c1-3-5-7-8-9-10-11-12-13-14-15-18-17(19)20-16-6-4-2/h2H,3,5-1

InchiKey: HCXDADQXPGQIHY-UHFFFAOYSA-N

Formula: C17H31NO2

SMILES: C#CCCOC(=O)NCCCCCCCCCCCC

Mol. weight [g/mol]: 281.43

Physical Properties

Property code	Value	Unit	Source
gf	170.80	kJ/mol	Joback Method
hf	-293.64	kJ/mol	Joback Method
hfus	50.65	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.657		Crippen Method
mcvol	259.210	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	704.94	K	Joback Method
tc	882.35	K	Joback Method
tf	453.14	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.55	J/mol×K	704.94	Joback Method
cpg	763.65	J/mol×K	734.51	Joback Method
cpg	779.92	J/mol×K	764.08	Joback Method
cpg	795.39	J/mol×K	793.65	Joback Method
cpg	810.09	J/mol×K	823.22	Joback Method
cpg	824.04	J/mol×K	852.79	Joback Method
cpg	837.25	J/mol×K	882.35	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=U415470&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