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

Inchi: InChI=1S/C13H23NO2/c1-3-5-7-8-9-10-11-14-13(15)16-12-6-4-2/h2H,3,5-12H2,1H3,(H,1

InchiKey: QFHHNHYYNSHSIW-UHFFFAOYSA-N

Formula: C13H23NO2

SMILES: C#CCCOC(=O)NCCCCCCCC

Mol. weight [g/mol]: 225.33

Physical Properties

Property code	Value	Unit	Source
gf	137.12	kJ/mol	Joback Method
hf	-211.08	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.096		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	613.42	K	Joback Method
tc	793.56	K	Joback Method
tf	408.06	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.57	J/mol×K	613.42	Joback Method
cpg	544.78	J/mol×K	643.44	Joback Method
cpg	559.29	J/mol×K	673.47	Joback Method
cpg	573.12	J/mol×K	703.49	Joback Method
cpg	586.28	J/mol×K	733.51	Joback Method
cpg	598.79	J/mol×K	763.53	Joback Method
cpg	610.68	J/mol×K	793.56	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=U415466&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

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