Carbonic acid, monoamide, N-2-ethylhexyl-, but-3-yn-1-yl ester

Inchi: InChI=1S/C13H23NO2/c1-4-7-9-12(6-3)11-14-13(15)16-10-8-5-2/h2,12H,4,6-11H2,1,3H3

InchiKey: XUPTYRDWCNUOHZ-UHFFFAOYSA-N

Formula: C13H23NO2

SMILES: C#CCCOC(=O)NCC(CC)CCCC

Mol. weight [g/mol]: 225.33

Physical Properties

Property code	Value	Unit	Source
gf	134.68	kJ/mol	Joback Method
hf	-216.36	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.952		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
tb	612.98	K	Joback Method
tc	796.19	K	Joback Method
tf	393.06	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.97	J/mol×K	612.98	Joback Method
cpg	545.48	J/mol×K	643.52	Joback Method
cpg	560.26	J/mol×K	674.05	Joback Method
cpg	574.33	J/mol×K	704.59	Joback Method
cpg	587.71	J/mol×K	735.12	Joback Method
cpg	600.40	J/mol×K	765.66	Joback Method
cpg	612.44	J/mol×K	796.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415464&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

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