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

Inchi: InChI=1S/C13H22O3/c1-3-5-7-8-9-10-12-16-13(14)15-11-6-4-2/h2H,3,5-12H2,1H3
InchiKey: SWQBNTUVYRSPOY-UHFFFAOYSA-N
Formula: C13H22O3
SMILES: C#CCCOC(=O)OCCCCCCCC
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-57.27	kJ/mol	Joback Method
hf	-396.77	kJ/mol	Joback Method
hfus	36.38	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.523		Crippen Method
mcvol	198.740	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
tb	585.67	K	Joback Method
tc	763.07	K	Joback Method
tf	377.63	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.56	J/mol×K	585.67	Joback Method
cpg	516.66	J/mol×K	615.24	Joback Method
cpg	531.12	J/mol×K	644.80	Joback Method
cpg	544.97	J/mol×K	674.37	Joback Method
cpg	558.20	J/mol×K	703.93	Joback Method
cpg	570.83	J/mol×K	733.50	Joback Method
cpg	582.86	J/mol×K	763.07	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383175&Units=SI

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