Carbonic acid, but-2-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/h3,5,7-12H2,1-2H3
InchiKey: ADESYSYBCIJCKU-UHFFFAOYSA-N
Formula: C13H22O3
SMILES: CC#CCOC(=O)OCCCCCCCC
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-77.54	kJ/mol	Joback Method
hf	-416.37	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.523		Crippen Method
mcvol	198.740	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	604.55	K	Joback Method
tc	790.21	K	Joback Method
tf	436.76	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.75	J/mol×K	604.55	Joback Method
cpg	520.36	J/mol×K	635.49	Joback Method
cpg	535.31	J/mol×K	666.44	Joback Method
cpg	549.60	J/mol×K	697.38	Joback Method
cpg	563.24	J/mol×K	728.32	Joback Method
cpg	576.22	J/mol×K	759.27	Joback Method
cpg	588.54	J/mol×K	790.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383204&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