Carbonic acid, but-2-yn-1-yl heptyl ester

Inchi: InChI=1S/C12H20O3/c1-3-5-7-8-9-11-15-12(13)14-10-6-4-2/h3,5,7-11H2,1-2H3
InchiKey: AAWSOYWONWMRIM-UHFFFAOYSA-N
Formula: C12H20O3
SMILES: CC#CCOC(=O)OCCCCCCC
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-85.96	kJ/mol	Joback Method
hf	-395.73	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.133		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
tb	581.67	K	Joback Method
tc	769.31	K	Joback Method
tf	425.49	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.50	J/mol×K	581.67	Joback Method
cpg	469.43	J/mol×K	612.94	Joback Method
cpg	483.74	J/mol×K	644.22	Joback Method
cpg	497.45	J/mol×K	675.49	Joback Method
cpg	510.54	J/mol×K	706.76	Joback Method
cpg	523.02	J/mol×K	738.04	Joback Method
cpg	534.89	J/mol×K	769.31	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=U383203&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume