Carbonic acid, di(but-2-yn-1-yl) ester

Inchi: InChI=1S/C9H10O3/c1-3-5-7-11-9(10)12-8-6-4-2/h7-8H2,1-2H3
InchiKey: HMKKBNWNSPLQFH-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CC#CCOC(=O)OCC#CC
Mol. weight [g/mol]: 166.17

Physical Properties

Property code	Value	Unit	Source
gf	91.58	kJ/mol	Joback Method
hf	-61.51	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.186		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	522.03	K	Joback Method
tc	742.25	K	Joback Method
tf	497.78	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.18	J/mol×K	522.03	Joback Method
cpg	290.34	J/mol×K	558.73	Joback Method
cpg	301.09	J/mol×K	595.44	Joback Method
cpg	311.42	J/mol×K	632.14	Joback Method
cpg	321.31	J/mol×K	668.85	Joback Method
cpg	330.74	J/mol×K	705.55	Joback Method
cpg	339.70	J/mol×K	742.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383215&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