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

Inchi: InChI=1S/C9H14O3/c1-4-5-6-11-9(10)12-7-8(2)3/h8H,6-7H2,1-3H3
InchiKey: FSROIPWWJDBLQB-UHFFFAOYSA-N
Formula: C9H14O3
SMILES: CC#CCOC(=O)OCC(C)C
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
gf	-113.66	kJ/mol	Joback Method
hf	-339.09	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	48.96	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.819		Crippen Method
mcvol	142.380	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
tb	512.59	K	Joback Method
tc	711.48	K	Joback Method
tf	376.68	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.54	J/mol×K	512.59	Joback Method
cpg	327.11	J/mol×K	545.74	Joback Method
cpg	339.23	J/mol×K	578.89	Joback Method
cpg	350.87	J/mol×K	612.03	Joback Method
cpg	362.04	J/mol×K	645.18	Joback Method
cpg	372.72	J/mol×K	678.33	Joback Method
cpg	382.90	J/mol×K	711.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383200&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