Carbonic acid, propargyl cyclohexylmethyl ester

Inchi: InChI=1S/C11H16O3/c1-2-8-13-11(12)14-9-10-6-4-3-5-7-10/h1,10H,3-9H2
InchiKey: WAOBZPLANFGHBU-UHFFFAOYSA-N
Formula: C11H16O3
SMILES: C#CCOC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 196.24

Physical Properties

Property code	Value	Unit	Source
gf	-49.66	kJ/mol	Joback Method
hf	-301.17	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.353		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
tb	559.46	K	Joback Method
tc	773.75	K	Joback Method
tf	362.47	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.08	J/mol×K	559.46	Joback Method
cpg	409.13	J/mol×K	595.18	Joback Method
cpg	425.26	J/mol×K	630.89	Joback Method
cpg	440.48	J/mol×K	666.61	Joback Method
cpg	454.80	J/mol×K	702.32	Joback Method
cpg	468.23	J/mol×K	738.04	Joback Method
cpg	480.78	J/mol×K	773.75	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=U357910&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