Carbonic acid, but-3-yn-1-yl isohexyl ester

Inchi: InChI=1S/C11H18O3/c1-4-5-8-13-11(12)14-9-6-7-10(2)3/h1,10H,5-9H2,2-3H3
InchiKey: LEOVYGPHDGNOBT-UHFFFAOYSA-N
Formula: C11H18O3
SMILES: C#CCCOC(=O)OCCCC(C)C
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-76.55	kJ/mol	Joback Method
hf	-360.77	kJ/mol	Joback Method
hfus	27.67	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.599		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	539.47	K	Joback Method
tc	723.67	K	Joback Method
tf	340.09	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.45	J/mol×K	539.47	Joback Method
cpg	418.40	J/mol×K	570.17	Joback Method
cpg	431.78	J/mol×K	600.87	Joback Method
cpg	444.60	J/mol×K	631.57	Joback Method
cpg	456.86	J/mol×K	662.27	Joback Method
cpg	468.57	J/mol×K	692.97	Joback Method
cpg	479.72	J/mol×K	723.67	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=U383173&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