Carbonic acid, hexyl prop-1-en-2-yl ester

Inchi: InChI=1S/C10H18O3/c1-4-5-6-7-8-12-10(11)13-9(2)3/h2,4-8H2,1,3H3
InchiKey: ZCXHXQBESVXQGM-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: C=C(C)OC(=O)OCCCCCC
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-226.31	kJ/mol	Joback Method
hf	-511.11	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.253		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1216.00		NIST Webbook
tb	523.47	K	Joback Method
tc	701.26	K	Joback Method
tf	281.13	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.14	J/mol×K	523.47	Joback Method
cpg	388.73	J/mol×K	553.10	Joback Method
cpg	401.81	J/mol×K	582.73	Joback Method
cpg	414.37	J/mol×K	612.36	Joback Method
cpg	426.43	J/mol×K	641.99	Joback Method
cpg	437.99	J/mol×K	671.62	Joback Method
cpg	449.04	J/mol×K	701.26	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=U382542&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume