Carbonic acid, but-3-en-1-yl hexyl ester

Inchi: InChI=1S/C11H20O3/c1-3-5-7-8-10-14-11(12)13-9-6-4-2/h4H,2-3,5-10H2,1H3
InchiKey: DEHFDEBDQQOIHH-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: C=CCCOC(=O)OCCCCCC
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-209.34	kJ/mol	Joback Method
hf	-521.96	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	50.98	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.296		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
tb	546.47	K	Joback Method
tc	719.93	K	Joback Method
tf	306.36	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.56	J/mol×K	546.47	Joback Method
cpg	436.77	J/mol×K	575.38	Joback Method
cpg	450.44	J/mol×K	604.29	Joback Method
cpg	463.57	J/mol×K	633.20	Joback Method
cpg	476.16	J/mol×K	662.11	Joback Method
cpg	488.21	J/mol×K	691.02	Joback Method
cpg	499.74	J/mol×K	719.93	Joback Method
dvisc	0.0021653	Pa×s	306.36	Joback Method

dvisc	0.0011102	Pa×s	346.38	Joback Method
dvisc	0.0006537	Pa×s	386.40	Joback Method
dvisc	0.0004251	Pa×s	426.42	Joback Method
dvisc	0.0002977	Pa×s	466.43	Joback Method
dvisc	0.0002205	Pa×s	506.45	Joback Method
dvisc	0.0001707	Pa×s	546.47	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=U383227&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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