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

Inchi: InChI=1S/C11H20O3/c1-4-5-8-13-11(12)14-9-6-7-10(2)3/h4,10H,1,5-9H2,2-3H3
InchiKey: UTKGOJDYDMHHCA-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: C=CCCOC(=O)OCCCC(C)C
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-211.78	kJ/mol	Joback Method
hf	-527.24	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	50.59	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	3.152		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
tb	546.03	K	Joback Method
tc	722.74	K	Joback Method
tf	291.36	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.86	J/mol×K	546.03	Joback Method
cpg	437.39	J/mol×K	575.48	Joback Method
cpg	451.36	J/mol×K	604.93	Joback Method
cpg	464.75	J/mol×K	634.38	Joback Method
cpg	477.59	J/mol×K	663.84	Joback Method
cpg	489.86	J/mol×K	693.29	Joback Method
cpg	501.56	J/mol×K	722.74	Joback Method
dvisc	0.0029039	Pa×s	291.36	Joback Method

dvisc	0.0013185	Pa×s	333.81	Joback Method
dvisc	0.0007154	Pa×s	376.25	Joback Method
dvisc	0.0004394	Pa×s	418.69	Joback Method
dvisc	0.0002952	Pa×s	461.14	Joback Method
dvisc	0.0002121	Pa×s	503.58	Joback Method
dvisc	0.0001604	Pa×s	546.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383226&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
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