Ethyl 4-methylpentan-2-yl carbonate

Inchi: InChI=1S/C9H18O3/c1-5-11-9(10)12-8(4)6-7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: CKVPXYFKQTVVGZ-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCOC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-318.90	kJ/mol	Joback Method
hf	-616.67	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.594		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
tb	503.15	K	Joback Method
tc	683.44	K	Joback Method
tf	255.58	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.47	J/mol×K	503.15	Joback Method
cpg	362.21	J/mol×K	533.20	Joback Method
cpg	375.46	J/mol×K	563.25	Joback Method
cpg	388.22	J/mol×K	593.29	Joback Method
cpg	400.49	J/mol×K	623.34	Joback Method
cpg	412.26	J/mol×K	653.39	Joback Method
cpg	423.52	J/mol×K	683.44	Joback Method
dvisc	0.0048998	Pa×s	255.58	Joback Method

dvisc	0.0019187	Pa×s	296.84	Joback Method
dvisc	0.0009445	Pa×s	338.10	Joback Method
dvisc	0.0005424	Pa×s	379.37	Joback Method
dvisc	0.0003473	Pa×s	420.63	Joback Method
dvisc	0.0002409	Pa×s	461.89	Joback Method
dvisc	0.0001774	Pa×s	503.15	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=U373801&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