Carbonic acid, allyl 2-methylbutyl ester

Inchi: InChI=1S/C9H16O3/c1-4-6-11-9(10)12-7-8(3)5-2/h4,8H,1,5-7H2,2-3H3
InchiKey: VQDIHNYHANVRTM-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: C=CCOC(=O)OCC(C)CC
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-228.62	kJ/mol	Joback Method
hf	-485.96	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	46.14	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.372		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
tb	500.27	K	Joback Method
tc	680.31	K	Joback Method
tf	268.82	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.15	J/mol×K	500.27	Joback Method
cpg	342.96	J/mol×K	530.28	Joback Method
cpg	355.30	J/mol×K	560.28	Joback Method
cpg	367.16	J/mol×K	590.29	Joback Method
cpg	378.56	J/mol×K	620.30	Joback Method
cpg	389.49	J/mol×K	650.31	Joback Method
cpg	399.94	J/mol×K	680.31	Joback Method
dvisc	0.0031058	Pa×s	268.82	Joback Method

dvisc	0.0014573	Pa×s	307.40	Joback Method
dvisc	0.0008095	Pa×s	345.97	Joback Method
dvisc	0.0005060	Pa×s	384.55	Joback Method
dvisc	0.0003445	Pa×s	423.12	Joback Method
dvisc	0.0002502	Pa×s	461.69	Joback Method
dvisc	0.0001908	Pa×s	500.27	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=U357376&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