Acetic acid, 1-tert-butoxyprop-2-yl ester

Inchi: InChI=1S/C9H18O3/c1-7(12-8(2)10)6-11-9(3,4)5/h7H,6H2,1-5H3
InchiKey: JEIHSRORUWXJGF-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CC(=O)OC(C)COC(C)(C)C
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-313.62	kJ/mol	Joback Method
hf	-620.14	kJ/mol	Joback Method
hfus	12.10	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.753		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1045.00		NIST Webbook
tb	500.36	K	Joback Method
tc	687.53	K	Joback Method
tf	273.00	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.24	J/mol×K	500.36	Joback Method
cpg	365.66	J/mol×K	531.56	Joback Method
cpg	379.45	J/mol×K	562.75	Joback Method
cpg	392.62	J/mol×K	593.95	Joback Method
cpg	405.18	J/mol×K	625.14	Joback Method
cpg	417.14	J/mol×K	656.34	Joback Method
cpg	428.51	J/mol×K	687.53	Joback Method
dvisc	0.0044878	Pa×s	273.00	Joback Method
dvisc	0.0018988	Pa×s	310.89	Joback Method

dvisc	0.0009684	Pa×s	348.79	Joback Method
dvisc	0.0005636	Pa×s	386.68	Joback Method
dvisc	0.0003613	Pa×s	424.57	Joback Method
dvisc	0.0002491	Pa×s	462.47	Joback Method
dvisc	0.0001817	Pa×s	500.36	Joback Method

Sources

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=U368957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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