Propanoic acid, 2,2-dimethyl, 1,1-dimethylethyl ester

Other names: tert-butyl pivalate
Inchi: InChI=1S/C9H18O2/c1-8(2,3)7(10)11-9(4,5)6/h1-6H3
InchiKey: VXHFNALHLRWIIU-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CC(C)(C)OC(=O)C(C)(C)C
Mol. weight [g/mol]: 158.24
CAS: 16474-43-4

Physical Properties

Property code	Value	Unit	Source
gf	-203.34	kJ/mol	Joback Method
hf	-491.39	kJ/mol	Joback Method
hfus	7.03	kJ/mol	Joback Method
hvap	42.19	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
ripol	939.00		NIST Webbook
tb	438.15 ± 2.50	K	NIST Webbook
tc	671.02	K	Joback Method
tf	268.19	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.36	J/mol×K	475.15	Joback Method
cpg	398.08	J/mol×K	638.37	Joback Method
cpg	385.75	J/mol×K	605.73	Joback Method
cpg	372.64	J/mol×K	573.08	Joback Method
cpg	358.74	J/mol×K	540.44	Joback Method

cpg	343.99	J/mol×K	507.79	Joback Method
cpg	409.69	J/mol×K	671.02	Joback Method
dvisc	0.0002365	Pa×s	475.15	Joback Method
dvisc	0.0003292	Pa×s	440.66	Joback Method
dvisc	0.0004847	Pa×s	406.16	Joback Method
dvisc	0.0007668	Pa×s	371.67	Joback Method
dvisc	0.0013324	Pa×s	337.18	Joback Method
dvisc	0.0026257	Pa×s	302.68	Joback Method
dvisc	0.0061612	Pa×s	268.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16474434&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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