

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

Inchi:	InChI=1S/C8H16O3/c1-7(10-6-9)5-11-8(2,3)4/h6-7H,5H2,1-4H3
InchiKey:	GHCHXRKSYDOKEP-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CC(COC(C)(C)C)OC=O
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-292.64	kJ/mol	Joback Method
hf	-572.50	kJ/mol	Joback Method
hfus	10.20	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.363		Crippen Method
mvol	136.890	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	980.00		NIST Webbook
tb	472.27	K	Joback Method
tc	656.76	K	Joback Method
tf	253.80	K	Joback Method
vc	0.519	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.97	J/molxK	472.27	Joback Method
cpg	368.07	J/molxK	626.01	Joback Method
cpg	357.12	J/molxK	595.27	Joback Method
cpg	345.65	J/molxK	564.52	Joback Method
cpg	333.63	J/molxK	533.77	Joback Method
cpg	321.08	J/molxK	503.02	Joback Method
cpg	378.50	J/molxK	656.76	Joback Method
dvisc	0.0002194	Paxs	472.27	Joback Method
dvisc	0.0003005	Paxs	435.86	Joback Method

dvisc	0.0004359	Paxs	399.45	Joback Method
dvisc	0.0006813	Paxs	363.03	Joback Method
dvisc	0.0011765	Paxs	326.62	Joback Method
dvisc	0.0023300	Paxs	290.21	Joback Method
dvisc	0.0056141	Paxs	253.80	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=U368956&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

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