Formic acid, 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C9H18O2/c1-8(6-11-7-10)5-9(2,3)4/h7-8H,5-6H2,1-4H3
InchiKey: RVKSKVZDYHFUFB-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CC(COC=O)CC(C)(C)C
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
gf	-179.22	kJ/mol	Joback Method
hf	-460.92	kJ/mol	Joback Method
hfus	11.61	kJ/mol	Joback Method
hvap	43.07	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.232		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1007.00		NIST Webbook
tb	472.73	K	Joback Method
tc	656.21	K	Joback Method
tf	242.84	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.63	J/mol×K	472.73	Joback Method
cpg	392.10	J/mol×K	625.63	Joback Method
cpg	380.26	J/mol×K	595.05	Joback Method
cpg	367.81	J/mol×K	564.47	Joback Method
cpg	354.74	J/mol×K	533.89	Joback Method
cpg	341.02	J/mol×K	503.31	Joback Method
cpg	403.35	J/mol×K	656.21	Joback Method
dvisc	0.0002453	Pa×s	472.73	Joback Method
dvisc	0.0003401	Pa×s	434.41	Joback Method

dvisc	0.0005023	Pa×s	396.10	Joback Method
dvisc	0.0008064	Pa×s	357.78	Joback Method
dvisc	0.0014502	Pa×s	319.47	Joback Method
dvisc	0.0030606	Pa×s	281.15	Joback Method
dvisc	0.0081761	Pa×s	242.84	Joback Method

Sources

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=U368952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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