Formic acid, 2-propylpentyl ester

Inchi: InChI=1S/C9H18O2/c1-3-5-9(6-4-2)7-11-8-10/h8-9H,3-7H2,1-2H3
InchiKey: YJTVTUBINXBKBA-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCC(CCC)COC=O
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
gf	-182.06	kJ/mol	Joback Method
hf	-452.17	kJ/mol	Joback Method
hfus	19.02	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1084.00		NIST Webbook
rinpol	1084.00		NIST Webbook
tb	475.96	K	Joback Method
tc	648.93	K	Joback Method
tf	240.42	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.93	J/mol×K	475.96	Joback Method
cpg	385.36	J/mol×K	620.10	Joback Method
cpg	374.02	J/mol×K	591.27	Joback Method
cpg	362.22	J/mol×K	562.44	Joback Method
cpg	349.94	J/mol×K	533.62	Joback Method
cpg	337.17	J/mol×K	504.79	Joback Method
cpg	396.23	J/mol×K	648.93	Joback Method
dvisc	0.0002462	Pa×s	475.96	Joback Method

dvisc	0.0003274	Pa×s	436.70	Joback Method
dvisc	0.0004608	Pa×s	397.45	Joback Method
dvisc	0.0006989	Pa×s	358.19	Joback Method
dvisc	0.0011744	Pa×s	318.93	Joback Method
dvisc	0.0022829	Pa×s	279.68	Joback Method
dvisc	0.0055140	Pa×s	240.42	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=U368748&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