Formic acid, 3-methylhept-3-yl ester

Inchi: InChI=1S/C9H18O2/c1-4-6-7-9(3,5-2)11-8-10/h8H,4-7H2,1-3H3
InchiKey: XRGVQQICCUIZMF-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCC(C)(CC)OC=O
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
gf	-176.78	kJ/mol	Joback Method
hf	-455.64	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	43.46	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.518		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1049.00		NIST Webbook
tb	473.17	K	Joback Method
tc	652.76	K	Joback Method
tf	257.84	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.49	J/mol×K	473.17	Joback Method
cpg	340.50	J/mol×K	503.10	Joback Method
cpg	353.87	J/mol×K	533.03	Joback Method
cpg	366.64	J/mol×K	562.96	Joback Method
cpg	378.81	J/mol×K	592.90	Joback Method
cpg	390.40	J/mol×K	622.83	Joback Method
cpg	401.43	J/mol×K	652.76	Joback Method
dvisc	0.0053072	Pa×s	257.84	Joback Method
dvisc	0.0023567	Pa×s	293.73	Joback Method

dvisc	0.0012489	Pa×s	329.62	Joback Method
dvisc	0.0007497	Pa×s	365.50	Joback Method
dvisc	0.0004931	Pa×s	401.39	Joback Method
dvisc	0.0003474	Pa×s	437.28	Joback Method
dvisc	0.0002581	Pa×s	473.17	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=U368949&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