Formic acid, 4-methylpent-2-yl ester

Inchi: InChI=1S/C7H14O2/c1-6(2)4-7(3)9-5-8/h5-7H,4H2,1-3H3
InchiKey: VJKXDWCVZONWBR-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CC(C)CC(C)OC=O
Mol. weight [g/mol]: 130.18

Physical Properties

Property code	Value	Unit	Source
gf	-201.34	kJ/mol	Joback Method
hf	-416.17	kJ/mol	Joback Method
hfus	10.32	kJ/mol	Joback Method
hvap	39.53	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.594		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	828.00		NIST Webbook
tb	429.76	K	Joback Method
tc	609.26	K	Joback Method
tf	202.88	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.27	J/mol×K	429.76	Joback Method
cpg	293.40	J/mol×K	579.34	Joback Method
cpg	283.58	J/mol×K	549.42	Joback Method
cpg	273.35	J/mol×K	519.51	Joback Method
cpg	262.72	J/mol×K	489.59	Joback Method
cpg	251.70	J/mol×K	459.68	Joback Method
cpg	302.84	J/mol×K	609.26	Joback Method
dvisc	0.0002613	Pa×s	429.76	Joback Method
dvisc	0.0003547	Pa×s	391.95	Joback Method

dvisc	0.0005137	Pa×s	354.13	Joback Method
dvisc	0.0008130	Pa×s	316.32	Joback Method
dvisc	0.0014574	Pa×s	278.51	Joback Method
dvisc	0.0031385	Pa×s	240.69	Joback Method
dvisc	0.0089962	Pa×s	202.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367940&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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