Formic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C6H12O2/c1-5(2)6(3)8-4-7/h4-6H,1-3H3
InchiKey: XEQSPMCNFJQDHU-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC(C)C(C)OC=O
Mol. weight [g/mol]: 116.16

Physical Properties

Property code	Value	Unit	Source
gf	-209.76	kJ/mol	Joback Method
hf	-395.53	kJ/mol	Joback Method
hfus	7.73	kJ/mol	Joback Method
hvap	37.30	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.204		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	763.00		NIST Webbook
tb	406.88	K	Joback Method
tc	587.63	K	Joback Method
tf	191.61	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.71	J/mol×K	406.88	Joback Method
cpg	211.86	J/mol×K	437.00	Joback Method
cpg	221.67	J/mol×K	467.13	Joback Method
cpg	231.14	J/mol×K	497.25	Joback Method
cpg	240.27	J/mol×K	527.38	Joback Method
cpg	249.06	J/mol×K	557.50	Joback Method
cpg	257.51	J/mol×K	587.63	Joback Method
dvisc	0.0088875	Pa×s	191.61	Joback Method
dvisc	0.0031355	Pa×s	227.49	Joback Method

dvisc	0.0014693	Pa×s	263.37	Joback Method
dvisc	0.0008258	Pa×s	299.25	Joback Method
dvisc	0.0005250	Pa×s	335.12	Joback Method
dvisc	0.0003644	Pa×s	371.00	Joback Method
dvisc	0.0002697	Pa×s	406.88	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=U367952&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