2-METHYLPENTYL FORMATE

Other names: Formic acid, 2-methylpentyl ester
Inchi: InChI=1S/C7H14O2/c1-3-4-7(2)5-9-6-8/h6-7H,3-5H2,1-2H3
InchiKey: KYHHSTLLLQRFHJ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC(C)COC=O
Mol. weight [g/mol]: 130.18
CAS: 381670-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-198.90	kJ/mol	Joback Method
hf	-410.89	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	39.92	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	898.00		NIST Webbook
rinpol	898.00		NIST Webbook
tb	430.20	K	Joback Method
tc	605.74	K	Joback Method
tf	217.88	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.20	J/mol×K	430.20	Joback Method
cpg	251.30	J/mol×K	459.46	Joback Method
cpg	262.02	J/mol×K	488.71	Joback Method
cpg	272.36	J/mol×K	517.97	Joback Method
cpg	282.32	J/mol×K	547.23	Joback Method
cpg	291.91	J/mol×K	576.48	Joback Method

cpg	301.13	J/mol×K	605.74	Joback Method
dvisc	0.0054507	Pa×s	217.88	Joback Method
dvisc	0.0023348	Pa×s	253.27	Joback Method
dvisc	0.0012312	Pa×s	288.65	Joback Method
dvisc	0.0007466	Pa×s	324.04	Joback Method
dvisc	0.0004996	Pa×s	359.43	Joback Method
dvisc	0.0003593	Pa×s	394.81	Joback Method
dvisc	0.0002728	Pa×s	430.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58072e+01
Coeff. B	-3.99047e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	314.52
Temperature range (K), max.	437.59

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C381670344&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume