Formic acid, hex-3-yl ester

Inchi: InChI=1S/C7H14O2/c1-3-5-7(4-2)9-6-8/h6-7H,3-5H2,1-2H3
InchiKey: YNOKGTVZHVEGIF-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC(CC)OC=O
Mol. weight [g/mol]: 130.18

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	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	872.00		NIST Webbook
rinpol	872.00		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

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=U367944&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

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