

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
mvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	872.00		NIST Webbook
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tb	430.20	K	Joback Method
tc	605.74	K	Joback Method
tf	217.88	K	Joback Method
vc	0.457	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.20	J/molxK	430.20	Joback Method
cpg	251.30	J/molxK	459.46	Joback Method
cpg	262.02	J/molxK	488.71	Joback Method
cpg	272.36	J/molxK	517.97	Joback Method
cpg	282.32	J/molxK	547.23	Joback Method
cpg	291.91	J/molxK	576.48	Joback Method
cpg	301.13	J/molxK	605.74	Joback Method
dvisc	0.0054507	Paxs	217.88	Joback Method

dvisc	0.0023348	Paxs	253.27	Joback Method
dvisc	0.0012312	Paxs	288.65	Joback Method
dvisc	0.0007466	Paxs	324.04	Joback Method
dvisc	0.0004996	Paxs	359.43	Joback Method
dvisc	0.0003593	Paxs	394.81	Joback Method
dvisc	0.0002728	Paxs	430.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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