

Formic acid, 5-methylhex-2-yl ester

Inchi:	InChI=1S/C8H16O2/c1-7(2)4-5-8(3)10-6-9/h6-8H,4-5H2,1-3H3
InchiKey:	KBIUZYHWAWGQLP-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CC(C)CCC(C)OC=O
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	-192.92	kJ/mol	Joback Method
hf	-436.81	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	41.76	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	956.00		NIST Webbook
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tb	452.64	K	Joback Method
tc	630.73	K	Joback Method
tf	214.15	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.09	J/molxK	452.64	Joback Method
cpg	293.67	J/molxK	482.32	Joback Method
cpg	305.79	J/molxK	512.00	Joback Method
cpg	317.45	J/molxK	541.69	Joback Method
cpg	328.65	J/molxK	571.37	Joback Method
cpg	339.41	J/molxK	601.05	Joback Method
cpg	349.72	J/molxK	630.73	Joback Method
dvisc	0.0089090	Paxs	214.15	Joback Method

dvisc	0.0030774	Paxs	253.90	Joback Method
dvisc	0.0014174	Paxs	293.65	Joback Method
dvisc	0.0007854	Paxs	333.39	Joback Method
dvisc	0.0004936	Paxs	373.14	Joback Method
dvisc	0.0003392	Paxs	412.89	Joback Method
dvisc	0.0002489	Paxs	452.64	Joback Method

Sources

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=U368887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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