

(Z)-2-Hexenyl formate

Inchi:	InChI=1S/C7H12O2/c1-2-3-4-5-6-9-7-8/h4-5,7H,2-3,6H2,1H3/b5-4-
InchiKey:	SLWYMCAVYPZTRN-PLNGDYQASA-N
Formula:	C7H12O2
SMILES:	CCCC=CCOC=O
Mol. weight [g/mol]:	128.17

Physical Properties

Property code	Value	Unit	Source
gf	-116.24	kJ/mol	Joback Method
hf	-288.39	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mvol	112.630	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	903.00		NIST Webbook
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tb	434.80	K	Joback Method
tc	614.89	K	Joback Method
tf	227.80	K	Joback Method
vc	0.443	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.30	J/molxK	434.80	Joback Method
cpg	234.73	J/molxK	464.82	Joback Method
cpg	244.75	J/molxK	494.83	Joback Method
cpg	254.34	J/molxK	524.85	Joback Method
cpg	263.54	J/molxK	554.86	Joback Method
cpg	272.34	J/molxK	584.88	Joback Method
cpg	280.76	J/molxK	614.89	Joback Method
dvisc	0.0032988	Paxs	227.80	Joback Method

dvisc	0.0015932	Paxs	262.30	Joback Method
dvisc	0.0009113	Paxs	296.80	Joback Method
dvisc	0.0005856	Paxs	331.30	Joback Method
dvisc	0.0004090	Paxs	365.80	Joback Method
dvisc	0.0003039	Paxs	400.30	Joback Method
dvisc	0.0002367	Paxs	434.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R98391&Units=SI
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

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
mccvol:	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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