3-hexenylformate

Other names: 3-Hexen-1-ol, formate
hex-3-enyl formate
Inchi: InChI=1S/C7H12O2/c1-2-3-4-5-6-9-7-8/h3-4,7H,2,5-6H2,1H3/b4-3+
InchiKey: XJHQVZQZUGLZLS-ONEGZZNKSA-N
Formula: C7H12O2
SMILES: CCC=CCCOC=O
Mol. weight [g/mol]: 128.17
CAS: 2315-09-5

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
mcvol	112.630	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	913.90		NIST Webbook
ripol	1416.00		NIST Webbook
tb	434.80	K	Joback Method
tc	614.89	K	Joback Method
tf	227.80	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.30	J/mol×K	434.80	Joback Method
cpg	234.73	J/mol×K	464.82	Joback Method
cpg	244.75	J/mol×K	494.83	Joback Method
cpg	254.34	J/mol×K	524.85	Joback Method
cpg	263.54	J/mol×K	554.86	Joback Method

cpg	272.34	J/mol×K	584.88	Joback Method
cpg	280.76	J/mol×K	614.89	Joback Method
dvisc	0.0032988	Pa×s	227.80	Joback Method
dvisc	0.0015932	Pa×s	262.30	Joback Method
dvisc	0.0009113	Pa×s	296.80	Joback Method
dvisc	0.0005856	Pa×s	331.30	Joback Method
dvisc	0.0004090	Pa×s	365.80	Joback Method
dvisc	0.0003039	Pa×s	400.30	Joback Method
dvisc	0.0002367	Pa×s	434.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2315095&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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