

# hexyl 5-hexenoate

<b>Inchi:</b>	InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h4H,2-3,5-11H2,1H3
<b>InchiKey:</b>	JZTSLYZRPJXJS-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O2
<b>SMILES:</b>	C=CCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	198.30

## Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-410.38	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1644.00		NIST Webbook
tb	546.93	K	Joback Method
tc	719.58	K	Joback Method
tf	295.40	K	Joback Method
vc	0.713	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.34	J/molxK	546.93	Joback Method
cpg	514.06	J/molxK	690.81	Joback Method
cpg	501.31	J/molxK	662.03	Joback Method
cpg	487.98	J/molxK	633.26	Joback Method
cpg	474.05	J/molxK	604.48	Joback Method
cpg	459.51	J/molxK	575.71	Joback Method

cpg	526.24	J/mol×K	719.58	Joback Method
dvisc	0.0001931	Paxs	546.93	Joback Method
dvisc	0.0002516	Paxs	505.01	Joback Method
dvisc	0.0003439	Paxs	463.09	Joback Method
dvisc	0.0005002	Paxs	421.17	Joback Method
dvisc	0.0007904	Paxs	379.24	Joback Method
dvisc	0.0013996	Paxs	337.32	Joback Method
dvisc	0.0029144	Paxs	295.40	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R313669&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R313669&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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