

# 3Z-hexenyl-d2 proprionate

<b>Inchi:</b>	InChI=1S/C9H16O2/c1-3-5-6-7-8-11-9(10)4-2/h5-6H,3-4,7-8H2,1-2H3/b6-5-/i1D2
<b>InchiKey:</b>	LGTLDEUQCOJGFP-BQAWHLCESA-N
<b>Formula:</b>	C9H14D2O2
<b>SMILES:</b>	CCC=CCCOC(=O)CC
<b>Mol. weight [g/mol]:</b>	158.23

## Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
ripol	1383.00		NIST Webbook
tb	485.77	K	Joback Method
tc	667.32	K	Joback Method
tf	258.27	K	Joback Method
vc	0.543	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.02	J/molxK	485.77	Joback Method
cpg	318.93	J/molxK	516.03	Joback Method
cpg	331.30	J/molxK	546.29	Joback Method
cpg	343.15	J/molxK	576.54	Joback Method
cpg	354.47	J/molxK	606.80	Joback Method
cpg	365.29	J/molxK	637.06	Joback Method
cpg	375.62	J/molxK	667.32	Joback Method
dvisc	0.0030655	Paxs	258.27	Joback Method
dvisc	0.0014558	Paxs	296.19	Joback Method

dvisc	0.0008186	Paxs	334.10	Joback Method
dvisc	0.0005177	Paxs	372.02	Joback Method
dvisc	0.0003563	Paxs	409.94	Joback Method
dvisc	0.0002612	Paxs	447.85	Joback Method
dvisc	0.0002011	Paxs	485.77	Joback Method

## Sources

<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=R328804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328804&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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