

# 3Z-hexenyl-d3 hexanoate-d3

<b>Inchi:</b>	InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5,7H,3-4,6,8-11H2,1-2H3/b7-5
<b>InchiKey:</b>	RGACQXBDYBCJCY-LPTCPRSGSA-N
<b>Formula:</b>	C12H16D6O2
<b>SMILES:</b>	CCC=CCCOC(=O)CCCCC
<b>Mol. weight [g/mol]:</b>	204.34

## Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/molxK	554.41	Joback Method
cpg	461.06	J/molxK	583.82	Joback Method
cpg	475.72	J/molxK	613.24	Joback Method
cpg	489.74	J/molxK	642.65	Joback Method
cpg	503.13	J/molxK	672.07	Joback Method
cpg	515.92	J/molxK	701.48	Joback Method
cpg	528.11	J/molxK	730.90	Joback Method
dvisc	0.0028734	Paxs	292.08	Joback Method

dvisc	0.0012967	Paxs	335.80	Joback Method
dvisc	0.0007029	Paxs	379.52	Joback Method
dvisc	0.0004324	Paxs	423.25	Joback Method
dvisc	0.0002914	Paxs	466.97	Joback Method
dvisc	0.0002101	Paxs	510.69	Joback Method
dvisc	0.0001595	Paxs	554.41	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R328859&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328859&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>
<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>

## 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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