

# 3Z-hexenyl-d3 acetate

Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h4-5H,3,6-7H2,1-2H3/b5-4-/i1D3
InchiKey:	NPFV00AXDOBMCE-OLODORCRSA-N
Formula:	C8H11D3O2
SMILES:	CCC=CCCOC(C)=O
Mol. weight [g/mol]:	145.21

## Physical Properties

Property code	Value	Unit	Source
gf	-137.22	kJ/mol	Joback Method
hf	-336.03	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
ripol	1309.00		NIST Webbook
tb	462.89	K	Joback Method
tc	646.21	K	Joback Method
tf	247.00	K	Joback Method
vc	0.487	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.30	J/molxK	462.89	Joback Method
cpg	317.95	J/molxK	615.66	Joback Method
cpg	307.96	J/molxK	585.10	Joback Method
cpg	297.52	J/molxK	554.55	Joback Method
cpg	286.60	J/molxK	524.00	Joback Method
cpg	275.19	J/molxK	493.44	Joback Method
cpg	327.49	J/molxK	646.21	Joback Method
dvisc	0.0002123	Paxs	462.89	Joback Method
dvisc	0.0002744	Paxs	426.91	Joback Method

dvisc	0.0003717	Paxs	390.93	Joback Method
dvisc	0.0005355	Paxs	354.94	Joback Method
dvisc	0.0008378	Paxs	318.96	Joback Method
dvisc	0.0014687	Paxs	282.98	Joback Method
dvisc	0.0030324	Paxs	247.00	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=R328819&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328819&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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