

# pentyl-d3 acetate

Inchi:	InChI=1S/C7H14O2/c1-3-4-5-6-9-7(2)8/h3-6H2,1-2H3/i2D3
InchiKey:	PGMYKACGEOXYJE-BMSJAHLVSA-N
Formula:	C7H11D3O2
SMILES:	CCCCCOC(C)=O
Mol. weight [g/mol]:	133.20

## Physical Properties

Property code	Value	Unit	Source
gf	-225.86	kJ/mol	Joback Method
hf	-432.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.740		Crippen Method
mvol	116.930	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
ripol	1173.00		NIST Webbook
ripol	1173.00		NIST Webbook
tb	435.85	K	Joback Method
tc	612.24	K	Joback Method
tf	240.81	K	Joback Method
vc	0.452	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.65	J/molxK	435.85	Joback Method
cpg	249.76	J/molxK	465.25	Joback Method
cpg	260.50	J/molxK	494.65	Joback Method
cpg	270.86	J/molxK	524.04	Joback Method
cpg	280.85	J/molxK	553.44	Joback Method
cpg	290.48	J/molxK	582.84	Joback Method
cpg	299.73	J/molxK	612.24	Joback Method
dvisc	0.0031909	Paxs	240.81	Joback Method

dvisc	0.0016480	Paxs	273.32	Joback Method
dvisc	0.0009795	Paxs	305.82	Joback Method
dvisc	0.0006434	Paxs	338.33	Joback Method
dvisc	0.0004549	Paxs	370.84	Joback Method
dvisc	0.0003401	Paxs	403.34	Joback Method
dvisc	0.0002656	Paxs	435.85	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R329134&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R329134&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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