

# hexyl-d3 proprionate

<b>Inchi:</b>	InChI=1S/C9H18O2/c1-3-5-6-7-8-11-9(10)4-2/h3-8H2,1-2H3/i1D3
<b>InchiKey:</b>	GOKKOFHHJFGZHW-FIBGUPNXSA-N
<b>Formula:</b>	C9H15D3O2
<b>SMILES:</b>	CCCCCOC(=O)CC
<b>Mol. weight [g/mol]:</b>	161.26

## Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-473.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	481.61	K	Joback Method
tc	655.29	K	Joback Method
tf	263.35	K	Joback Method
vc	0.564	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	481.61	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	395.29	J/mol×K	655.29	Joback Method
dvisc	0.0033103	Paxs	263.35	Joback Method

dvisc	0.0016384	Paxs	299.73	Joback Method
dvisc	0.0009442	Paxs	336.10	Joback Method
dvisc	0.0006060	Paxs	372.48	Joback Method
dvisc	0.0004209	Paxs	408.86	Joback Method
dvisc	0.0003103	Paxs	445.23	Joback Method
dvisc	0.0002395	Paxs	481.61	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R329090&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R329090&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>mccvol:</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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