

# propyl hexanoate-d11

<b>Inchi:</b>	InChI=1S/C9H18O2/c1-3-5-6-7-9(10)11-8-4-2/h3-8H2,1-2H3/i1D3,3D2,5D2,6D2,7D2
<b>InchiKey:</b>	HTUIWRWYYVBCFT-LELBNVJRSA-N
<b>Formula:</b>	C9H7D11O2
<b>SMILES:</b>	CCCCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	169.31

## 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
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
ripol	1308.00		NIST Webbook
tb	481.61	K	Joback Method
tc	655.29	K	Joback Method
tf	263.35	K	Joback Method
vc	0.564	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/molxK	481.61	Joback Method
cpg	384.40	J/molxK	626.35	Joback Method
cpg	373.04	J/molxK	597.40	Joback Method
cpg	361.21	J/molxK	568.45	Joback Method
cpg	348.92	J/molxK	539.50	Joback Method
cpg	336.15	J/molxK	510.56	Joback Method
cpg	395.29	J/molxK	655.29	Joback Method
dvisc	0.0002395	Paxs	481.61	Joback Method
dvisc	0.0003103	Paxs	445.23	Joback Method

dvisc	0.0004209	Paxs	408.86	Joback Method
dvisc	0.0006060	Paxs	372.48	Joback Method
dvisc	0.0009442	Paxs	336.10	Joback Method
dvisc	0.0016384	Paxs	299.73	Joback Method
dvisc	0.0033103	Paxs	263.35	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=R329169&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R329169&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>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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