

# 2E-hexenol-d3

<b>Inchi:</b>	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h4-5,7H,2-3,6H2,1H3/b5-4+/i1D3
<b>InchiKey:</b>	ZCHHRLHTBGRGOT-TYYDCBDZSA-N
<b>Formula:</b>	C6H9D3O
<b>SMILES:</b>	CCCC=CCO
<b>Mol. weight [g/mol]:</b>	103.18

## Physical Properties

Property code	Value	Unit	Source
gf	-56.96	kJ/mol	Joback Method
hf	-202.18	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.335		Crippen Method
mvol	96.970	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
ripol	1409.00		NIST Webbook
ripol	1409.00		NIST Webbook
tb	433.02	K	Joback Method
tc	601.76	K	Joback Method
tf	213.12	K	Joback Method
vc	0.370	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.78	J/molxK	433.02	Joback Method
cpg	233.69	J/molxK	573.64	Joback Method
cpg	226.05	J/molxK	545.51	Joback Method
cpg	218.06	J/molxK	517.39	Joback Method
cpg	209.69	J/molxK	489.27	Joback Method
cpg	200.94	J/molxK	461.14	Joback Method
cpg	240.99	J/molxK	601.76	Joback Method
dvisc	0.0002006	Paxs	433.02	Joback Method

dvisc	0.0003473	Paxs	396.37	Joback Method
dvisc	0.0006726	Paxs	359.72	Joback Method
dvisc	0.0015133	Paxs	323.07	Joback Method
dvisc	0.0041899	Paxs	286.42	Joback Method
dvisc	0.0156415	Paxs	249.77	Joback Method
dvisc	0.0918576	Paxs	213.12	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=R328651&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328651&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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