

# 2E-hexenal-d3

<b>Inchi:</b>	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3/b5-4+/i1D3
<b>InchiKey:</b>	MBDOYVRWFFCFHM-TYYDCBDZSA-N
<b>Formula:</b>	C6H7D3O
<b>SMILES:</b>	CCCC=CC=O
<b>Mol. weight [g/mol]:</b>	101.16

## Physical Properties

Property code	Value	Unit	Source
gf	-19.66	kJ/mol	Joback Method
hf	-135.53	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
ripol	1202.00		NIST Webbook
tb	389.50	K	Joback Method
tc	570.95	K	Joback Method
tf	194.30	K	Joback Method
vc	0.368	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.69	J/molxK	389.50	Joback Method
cpg	174.16	J/molxK	419.74	Joback Method
cpg	183.18	J/molxK	449.98	Joback Method
cpg	191.76	J/molxK	480.23	Joback Method
cpg	199.93	J/molxK	510.47	Joback Method
cpg	207.70	J/molxK	540.71	Joback Method
cpg	215.09	J/molxK	570.95	Joback Method
dvisc	0.0038680	Paxs	194.30	Joback Method
dvisc	0.0017894	Paxs	226.83	Joback Method

dvisc	0.0010044	Paxs	259.37	Joback Method
dvisc	0.0006413	Paxs	291.90	Joback Method
dvisc	0.0004480	Paxs	324.43	Joback Method
dvisc	0.0003341	Paxs	356.97	Joback Method
dvisc	0.0002617	Paxs	389.50	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R328646&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328646&amp;Units=SI</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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