

# d3-2E-hexenyl 2-methylbutanoate

<b>Inchi:</b>	InChI=1S/C11H20O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h6-7,10H,4-5,8-9H2,1-3H3/b7-6+/i
<b>InchiKey:</b>	JKKGTSUICJWEKB-ZRNNCLBUSA-N
<b>Formula:</b>	C11H17D3O2
<b>SMILES:</b>	CCC=CCCOC(=O)C(C)CC
<b>Mol. weight [g/mol]:</b>	187.29

## Physical Properties

Property code	Value	Unit	Source
gf	-114.40	kJ/mol	Joback Method
hf	-403.23	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mvol	168.990	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
ripol	1477.00		NIST Webbook
ripol	1477.00		NIST Webbook
tb	531.09	K	Joback Method
tc	712.68	K	Joback Method
tf	265.81	K	Joback Method
vc	0.649	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.61	J/molxK	531.09	Joback Method
cpg	412.58	J/molxK	561.36	Joback Method
cpg	426.88	J/molxK	591.62	Joback Method
cpg	440.55	J/molxK	621.89	Joback Method
cpg	453.60	J/molxK	652.15	Joback Method
cpg	466.04	J/molxK	682.42	Joback Method
cpg	477.89	J/molxK	712.68	Joback Method
dvisc	0.0042170	Paxs	265.81	Joback Method

dvisc	0.0016682	Paxs	310.02	Joback Method
dvisc	0.0008318	Paxs	354.24	Joback Method
dvisc	0.0004840	Paxs	398.45	Joback Method
dvisc	0.0003138	Paxs	442.66	Joback Method
dvisc	0.0002201	Paxs	486.88	Joback Method
dvisc	0.0001638	Paxs	531.09	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=R328973&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R328973&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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