

# 2-Methyl-2-ethyl-3-hydroxyhexyl propionate

<b>Other names:</b>	2-methyl-2-ethyl-3 hydroxyhexyl propanoate
<b>Inchi:</b>	InChI=1S/C12H24O3/c1-5-8-10(13)12(4,7-3)9-15-11(14)6-2/h10,13H,5-9H2,1-4H3
<b>InchiKey:</b>	QONBAQBZDACBTM-UHFFFAOYSA-N
<b>Formula:</b>	C12H24O3
<b>SMILES:</b>	CCCC(O)C(C)(CC)COC(=O)CC
<b>Mol. weight [g/mol]:</b>	216.32

## Physical Properties

Property code	Value	Unit	Source
gf	-320.18	kJ/mol	Joback Method
hf	-702.07	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	66.46	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.517		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1378.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	1859.00		NIST Webbook
tb	638.76	K	Joback Method
tc	814.17	K	Joback Method
tf	345.40	K	Joback Method
vc	0.734	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.52	J/molxK	638.76	Joback Method
cpg	547.80	J/molxK	668.00	Joback Method
cpg	561.38	J/molxK	697.23	Joback Method
cpg	574.29	J/molxK	726.47	Joback Method
cpg	586.55	J/molxK	755.70	Joback Method
cpg	598.18	J/molxK	784.94	Joback Method

cpg	609.21	J/molxK	814.17	Joback Method
dvisc	0.0069125	Paxs	345.40	Joback Method
dvisc	0.0017625	Paxs	394.29	Joback Method
dvisc	0.0006075	Paxs	443.19	Joback Method
dvisc	0.0002588	Paxs	492.08	Joback Method
dvisc	0.0001286	Paxs	540.97	Joback Method
dvisc	0.0000718	Paxs	589.87	Joback Method
dvisc	0.0000438	Paxs	638.76	Joback Method

## Sources

<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=R331598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331598&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>

## 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>rinpol:</b>	Non-polar retention indices
<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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