

# 3-Hexen-1-ol, butanoate

<b>Other names:</b>	3-hexenyl butanoate butanoic acid, 3-hexenyl ester Hex-3-enyl butyrate hex-3-en-1-yl butanoate 3-Hexenyl butyrate hex-3-enyl butanoate
<b>Inchi:</b>	InChI=1S/C10H18O2/c1-3-5-6-7-9-12-10(11)8-4-2/h5-6H,3-4,7-9H2,1-2H3
<b>InchiKey:</b>	ZCHOPXVYTWUHDS-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	CCC=CCCOC(=O)CCC
<b>Mol. weight [g/mol]:</b>	170.25

## Physical Properties

Property code	Value	Unit	Source
gf	-120.38	kJ/mol	Joback Method
hf	-377.31	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1186.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1186.00		NIST Webbook
tb	508.65	K	Joback Method
tc	688.43	K	Joback Method
tf	269.54	K	Joback Method
vc	0.600	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.74	J/mol×K	508.65	Joback Method

cpg	414.10	J/mol×K	658.47	Joback Method
cpg	402.54	J/mol×K	628.50	Joback Method
cpg	390.44	J/mol×K	598.54	Joback Method
cpg	377.79	J/mol×K	568.58	Joback Method
cpg	364.56	J/mol×K	538.61	Joback Method
cpg	425.13	J/mol×K	688.43	Joback Method
dvisc	0.0001880	Paxs	508.65	Joback Method
dvisc	0.0002455	Paxs	468.80	Joback Method
dvisc	0.0003369	Paxs	428.95	Joback Method
dvisc	0.0004933	Paxs	389.10	Joback Method
dvisc	0.0007878	Paxs	349.24	Joback Method
dvisc	0.0014196	Paxs	309.39	Joback Method
dvisc	0.0030444	Paxs	269.54	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=R163736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R163736&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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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