

# methylpropyl-d3 butanoate-d3

<b>Inchi:</b>	InChI=1S/C8H16O2/c1-4-5-8(9)10-6-7(2)3/h7H,4-6H2,1-3H3/i1D3,2D3,4D2,5D2
<b>InchiKey:</b>	RGFNRWTDWVHDD-IZUSZFKNSA-N
<b>Formula:</b>	C8H6D10O2
<b>SMILES:</b>	CCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	154.27

## Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
ripol	1160.00		NIST Webbook
tb	458.29	K	Joback Method
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/molxK	458.29	Joback Method
cpg	292.41	J/molxK	488.10	Joback Method
cpg	304.54	J/molxK	517.91	Joback Method
cpg	316.22	J/molxK	547.72	Joback Method
cpg	327.44	J/molxK	577.53	Joback Method
cpg	338.23	J/molxK	607.34	Joback Method
cpg	348.57	J/molxK	637.16	Joback Method
dvisc	0.0048246	Paxs	237.08	Joback Method
dvisc	0.0020946	Paxs	273.95	Joback Method

dvisc	0.0011084	Paxs	310.82	Joback Method
dvisc	0.0006713	Paxs	347.69	Joback Method
dvisc	0.0004476	Paxs	384.55	Joback Method
dvisc	0.0003204	Paxs	421.42	Joback Method
dvisc	0.0002420	Paxs	458.29	Joback Method

## Sources

<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=R329114&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R329114&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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