

# Hexanoic acid, 2-butyl-

<b>Other names:</b>	2-Butylhexanoic acid Dibutylacetic acid Isocarb 10
<b>Inchi:</b>	InChI=1S/C10H20O2/c1-3-5-7-9(10(11)12)8-6-4-2/h9H,3-8H2,1-2H3,(H,11,12)
<b>InchiKey:</b>	KQYRYPXQPKPVSP-UHFFFAOYSA-N
<b>Formula:</b>	C10H20O2
<b>SMILES:</b>	CCCCC(CCCC)C([O])=O
<b>Mol. weight [g/mol]:</b>	172.26
<b>CAS:</b>	3115-28-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	2.940		Crippen Method
mcvol	157.050	ml/mol	McGowan 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=C3115284&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3115284&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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