

Butyric acid, 2-amino-, l-(+)-

Inchi:	InChI=1S/C4H9NO2/c1-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)/t3-/m1/s1
InchiKey:	QWCKQJZIFLGMSD-GSVOUGTGSA-N
Formula:	C4H9NO2
SMILES:	CCC([NH3+])C(=O)[O-]
Mol. weight [g/mol]:	103.12

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	-2.243		Crippen Method
mcvol	84.640	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008156&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/15-400-0/Butyric-acid-2-amino-l.pdf>

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