

DI-alpha-amino-n-caproic acid

Inchi:	InChI=1S/C6H13NO2/c1-2-3-4-5(7)6(8)9/h5H,2-4,7H2,1H3,(H,8,9)/t5-/m0/s1
InchiKey:	LRQKBLKVPFOOQJ-YFKPBYRVSA-N
Formula:	C6H13NO2
SMILES:	CCCCC([NH3+])C(=O)[O-]
Mol. weight [g/mol]:	131.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.71		Crippen Method
logp	-1.463		Crippen Method
mcvol	112.820	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=B6008974&Units=SI

Legend

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

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