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Typical Product Specifications & Properties

(S)-2-Acetamido-3-methylbutanoic acid

CAS Number: : 96-81-1

Specifications	Limits
Molecular weight	159.18
EINECS	202-537-8
SMILES	<chem>CC(=O)N[C@H](C(=O)O)C(C)C</chem>
InChI	1S/C7H13NO3/c1-4(2)6(7(10)11)8-5(3)9/h4,6H,1-3H3,(H,8,9)(H,10,11)/t6-m/s1
InChIKey	IHYJTAOFMMMOPX-LURJTMIESA-N
log P (octanol-water)	0.300
Atmospheric OH Rate Constant	1.62E-11 cm ³ /molecule-sec
Water solubility	6.95E+04 mg/L
Storage Temperature	-20°C
Melting Point	163-167?



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