2-Propenoic acid, 2-(acetylamino)-

Other names:	Acrylic acid, 2-acetamido- «alpha»-Acetamidoacrylic acid N-Acetyldehydroalanine 2-Acetamidoacrylic acid Acetyldehydroalanine 2-Acetamidocrylic acid
Inchi:	InChI=1S/C5H7NO3/c1-3(5(8)9)6-4(2)7/h1H2,2H3,(H,6,7)(H,8,9)
InchiKey:	UFDFFEMHDKXMBG-UHFFFAOYSA-N
Formula:	C5H7NO3
SMILES:	C=C(N=C(C)O)C(=O)O
Mol. weight [g/mol]:	129.11
CAS:	5429-56-1

Physical Properties

Property code	Value	Unit	Source
hf	-375.50	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
ie	8.88	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
log10ws	-0.35		Crippen Method
logp	0.561		Crippen Method
mcvol	96.000	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
tb	625.15	K	Joback Method
tc	814.50	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5429561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature