2-Butenoic acid, 2-(acetylamino)-

Inchi: InChI=1S/C6H9NO3/c1-3-5(6(9)10)7-4(2)8/h3H,1-2H3,(H,7,8)(H,9,10)/b5-3+
InchiKey: RZLLYKKORUSDSK-HWKANZROSA-N
Formula: C6H9NO3
SMILES: CC=C(NC(C)=O)C(=O)O
Mol. weight [g/mol]: 143.14
CAS: 55649-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-233.96	kJ/mol	Joback Method
hf	-383.66	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
ie	8.93	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-0.75		Crippen Method
logp	0.111		Crippen Method
mcvol	110.090	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	590.81	K	Joback Method
tc	783.30	K	Joback Method
tf	351.68	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.99	J/mol×K	590.81	Joback Method
cpg	265.98	J/mol×K	622.89	Joback Method
cpg	273.51	J/mol×K	654.97	Joback Method
cpg	280.61	J/mol×K	687.06	Joback Method
cpg	287.30	J/mol×K	719.14	Joback Method
cpg	293.59	J/mol×K	751.22	Joback Method
cpg	299.52	J/mol×K	783.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55649713&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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume