«alpha»-Acetamidocinnamic acid

Other names: «alpha»-Acetaminocinnamic acid
2-Propenoic acid, 2-(acetylamino)-3-phenyl-
«alpha»-Acetoamidocinnamic acid
3-Phenyl-2-acetylaminoprop-2-enoic acid
1-acetamidocinnamic acid
Inchi: InChI=1S/C11H11NO3/c1-8(13)12-10(11(14)15)7-9-5-3-2-4-6-9/h2-7H,1H3,(H,12,13)(H,
InchiKey: XODAOBAZOQSFDS-YFHOEESVSA-N
Formula: C11H11NO3
SMILES: CC(=O)NC(=Cc1ccccc1)C(=O)O
Mol. weight [g/mol]: 205.21
CAS: 5469-45-4

Physical Properties

Property code	Value	Unit	Source
gf	-79.45	kJ/mol	Joback Method
hf	-250.33	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
ie	8.67	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.11		Crippen Method
logp	1.248		Crippen Method
mcvol	156.780	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	731.89	K	Joback Method
tc	946.61	K	Joback Method
tf	434.45	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	412.19	J/mol×K	731.89	Joback Method
cpg	422.06	J/mol×K	767.68	Joback Method
cpg	431.21	J/mol×K	803.46	Joback Method
cpg	439.70	J/mol×K	839.25	Joback Method
cpg	447.57	J/mol×K	875.04	Joback Method
cpg	454.89	J/mol×K	910.83	Joback Method
cpg	461.70	J/mol×K	946.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5469454&Units=SI

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