(Z)-3-Phenyl-2-propenoic acid

Other names:	(2Z)-3-Phenyl-2-propenoic acid
	(Z)-3-phenylacrylic acid
	(Z)-cinnamic acid
	2-Propenoic acid, 3-phenyl-, (Z)-
	Allocinnamic acid
	Cinnamic acid, (Z)-
	Cinnamic acid, cis-
	Isocinnamic acid
	cis-cinnamic acid
	cis-«beta»-Carboxystyrene
Inchi:	InChI=1S/C9H8O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H,10,11)/b7-6-
InchiKey:	WBYWAXJHAXSJNI-SREVYHEPSA-N
Formula:	C9H8O2
SMILES:	O=C(O)C=Cc1ccccc1
Mol. weight [g/mol]:	148.16
CAS:	102-94-3

Physical Properties

Property code	Value	Unit	Source
chs	-4385.30	kJ/mol	NIST Webbook
chs	-4383.80 ± 1.70	kJ/mol	NIST Webbook
chs	-4366.00 ± 1.70	kJ/mol	NIST Webbook
chs	-4373.70 ± 1.70	kJ/mol	NIST Webbook
chs	-4368.00 ± 1.70	kJ/mol	NIST Webbook
gf	-48.21	kJ/mol	Joback Method
hf	-140.15	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	61.29	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-1.81		Crippen Method
logp	1.784		Crippen Method
mcvol	117.050	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
ripol	2735.00		NIST Webbook
tb	582.21	K	Joback Method
tc	794.16	K	Joback Method

tf	340.10	K	Energetics of neutral and deprotonated (Z)-cinnamic acid
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.73	J/mol×K	758.84	Joback Method
cpg	296.41	J/mol×K	723.51	Joback Method
cpg	288.54	J/mol×K	688.19	Joback Method
cpg	280.05	J/mol×K	652.86	Joback Method
cpg	270.92	J/mol×K	617.54	Joback Method
cpg	261.10	J/mol×K	582.21	Joback Method
cpg	310.53	J/mol×K	794.16	Joback Method
dvisc	0.0067351	Pa×s	323.28	Joback Method
dvisc	0.0000904	Pa×s	582.21	Joback Method
dvisc	0.0001391	Pa×s	539.06	Joback Method
dvisc	0.0002307	Pa×s	495.90	Joback Method
dvisc	0.0004214	Pa×s	452.75	Joback Method
dvisc	0.0008737	Pa×s	409.59	Joback Method
dvisc	0.0021509	Pa×s	366.44	Joback Method
hfust	16.95	kJ/mol	341.20	NIST Webbook
hfust	16.95	kJ/mol	341.20	NIST Webbook

Sources

Energetics of neutral and deprotonated (Z)-cinnamic acid: https://www.doi.org/10.1016/j.jct.2015.12.014
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=C102943&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume