trans-Cinnamic acid

Other names:	(2E)-3-Phenyl-2-propenoic acid (E)-3-Phenyl-2-propenoic acid (E)-3-Phenylacrylic acid (E)-cinnamic acid 2-Propenoic acid, 3-phenyl-, (2E)- 2-propenoic acid, 3-phenyl-, (E)- Cinnamic acid NSC 44010 cinnamic acid, (E)- trans-3-Phenyl-2-propenoic acid trans-3-phenylacrylic acid trans-3-phenylpropenoic acid trans-«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-VOTSOKGWSA-N
Formula:	C9H8O2
SMILES:	O=C(O)C=Cc1ccccc1
Mol. weight [g/mol]:	148.16
CAS:	140-10-3

Physical Properties

Property code	Value	Unit	Source
chs	-4344.70	kJ/mol	NIST Webbook
chs	-4348.00 ± 2.00	kJ/mol	NIST Webbook
chs	-4359.30	kJ/mol	NIST Webbook
gf	-48.21	kJ/mol	Joback Method
hf	-140.15	kJ/mol	Joback Method
hfs	-325.30	kJ/mol	NIST Webbook
hfs	-337.00	kJ/mol	NIST Webbook
hfs	-340.00	kJ/mol	NIST Webbook
hfus	19.00	kJ/mol	Joback Method
hsub	107.10 ± 0.80	kJ/mol	NIST Webbook
hvap	61.29	kJ/mol	Joback Method
ie	9.00 ± 0.05	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
rinpol	1428.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1450.90		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2804.00		NIST Webbook
ripol	2835.00		NIST Webbook
ripol	2827.00		NIST Webbook
ripol	2844.00		NIST Webbook
ripol	2842.00		NIST Webbook
ripol	2832.00		NIST Webbook
tb	573.20	K	NIST Webbook
tc	794.16	K	Joback Method
tf	406.15	K	Solid Liquid Phase Equilibrium of trans-Cinnamic Acid in Several Alcohols: Measurements and Thermodynamic Modeling
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.53	J/mol×K	794.16	Joback Method
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
cps	197.50	J/mol×K	323.00	NIST Webbook
dvisc	0.0002307	Pa×s	495.90	Joback Method

dvisc	0.0004214	Pa×s	452.75	Joback Method
dvisc	0.0000904	Pa×s	582.21	Joback Method
dvisc	0.0021509	Pa×s	366.44	Joback Method
dvisc	0.0067351	Pa×s	323.28	Joback Method
dvisc	0.0001391	Pa×s	539.06	Joback Method
dvisc	0.0008737	Pa×s	409.59	Joback Method
hfust	22.63	kJ/mol	406.15	NIST Webbook
hfust	22.21	kJ/mol	406.10	NIST Webbook
hfust	22.63	kJ/mol	406.20	NIST Webbook
hfust	22.60	kJ/mol	404.80	NIST Webbook
hvapt	73.90	kJ/mol	501.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of cinnamic acid in supercritical carbon dioxide and supercritical 1,1,1,2-tetrafluoroethane:	https://www.doi.org/10.1016/j.fluid.2018.10.009
Solid-Liquid Phase Equilibrium of trans-Cinnamic Acid in Several Alcohols: Measurements and Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.5b00814
Experimental Data and Modeling: Cinnamic Acid Solubility Enhancement in the Presence of Ethanol As a Supercritical CO2 Cosolvent:	https://www.doi.org/10.1021/je900154x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume