2-Propenoic acid, 3-phenyl-

Other names:	3-Phenyl-2-propenoic acid (cinnamic acid)
	3-phenyl-2-propenoic acid
	3-phenylacrylic acid
	3-phenylpropenoic acid
	Cinnamylic acid
	Kyselina skoricove
	NSC 9189
	Phenylacrylic acid
	Zimtsaeure
	beta-Phenylacrylic acid
	cinnamic acid
	«beta»-Phenylacrylic acid
Inchi:	InChI=1S/C9H8O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H,10,11)
InchiKey:	WBYWAXJHAXSJNI-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	O=C(O)C=Cc1ccccc1
Mol. weight [g/mol]:	148.16
CAS:	621-82-9

Physical Properties

Property code	Value	Unit	Source
chs	-4357.20	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
log10ws	-1.81		Crippen Method
logp	1.784		Crippen Method
mcvol	117.050	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1435.00		NIST Webbook

rinpol	1396.00		NIST Webbook
ripol	2801.00		NIST Webbook
ripol	2869.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2845.00		NIST Webbook
ripol	2830.00		NIST Webbook
ripol	2830.00		NIST Webbook
tb	582.21	K	Joback Method
tc	794.16	K	Joback Method
tf	406.15 ± 0.20	K	NIST Webbook
tf	406.15 ± 0.70	K	NIST Webbook
tf	410.00 ± 1.50	K	NIST Webbook
tf	406.00 ± 2.00	K	NIST Webbook
tf	406.30 ± 0.50	K	NIST Webbook
tf	406.00 ± 2.00	K	NIST Webbook
tf	406.00 ± 1.00	K	NIST Webbook
tf	406.35 ± 1.00	K	NIST Webbook
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of cinnamic acid, phenoxyacetic acid and 4-methoxyphenylacetic acid in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2008.09.009
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=C621829&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
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