

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	1435.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1434.00		NIST Webbook

ripol	1396.00		NIST Webbook
ripol	2845.00		NIST Webbook
ripol	2830.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2869.00		NIST Webbook
ripol	2801.00		NIST Webbook
ripol	2830.00		NIST Webbook
ripol	2852.00		NIST Webbook
tb	582.21	K	Joback Method
tc	794.16	K	Joback Method
tf	406.15 ± 0.20	K	NIST Webbook
tf	406.00 ± 2.00	K	NIST Webbook
tf	406.15 ± 0.70	K	NIST Webbook
tf	406.00 ± 1.00	K	NIST Webbook
tf	406.00 ± 2.00	K	NIST Webbook
tf	406.30 ± 0.50	K	NIST Webbook
tf	410.00 ± 1.50	K	NIST Webbook
tf	406.35 ± 1.00	K	NIST Webbook
vc	0.436	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Solubilities of cinnamic acid,
phenoxyacetic acid and
4-phenoxyphenylacetic acid in
supercritical carbon dioxide:
McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2008.09.009>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C621829&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
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

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