Hydrocinnamic acid

Other names:	.beta.-phenylpropionic acid
	3-Phenylpropanoic acid
	3-Phenylpropionic acid
	Benzenepropanoic acid
	Benzenepropionic acid
	Benzylacetic acid
	Dihydrocinnamic acid
	NSC 9272
	Phenylpropanoic acid
	Phenylpropionic acid
	propanoic acid, 3-phenyl-
	propionic acid, 3-phenyl-
	«beta»-Phenylpropanoic acid
	«beta»-Phenylpropionic acid
	Â«betaÂ»-Phenylpropanoic acid
	Â«betaÂ»-Phenylpropionic acid
Inchi:	InChI=1S/C9H10O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,11)
InchiKey:	XMIIGOLPHOKFCH-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	O=C(O)CCc1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	501-52-0

Physical Properties

Property code	Value	Unit	Source
gf	-128.43	kJ/mol	Joback Method
hf	-257.37	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hsub	102.40 ± 0.80	kJ/mol	NIST Webbook
hvap	61.33	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-1.41		Aqueous Solubility Prediction Method
logp	1.704		Crippen Method
mcvol	121.350	ml/mol	McGowan Method

pc	3460.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
rinpol	1344.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1366.50		NIST Webbook
rinpol	230.64		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	230.64		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2650.00		NIST Webbook
ripol	2635.00		NIST Webbook
ripol	2633.00		NIST Webbook
ripol	2608.00		NIST Webbook
ripol	2638.00		NIST Webbook
ripol	2650.00		NIST Webbook
ripol	2650.00		NIST Webbook
tb	553.00	K	NIST Webbook
tc	781.24	K	Joback Method
tf	321.00 ± 1.50	K	NIST Webbook
tf	333.65	K	Aqueous Solubility Prediction Method
tf	321.15 ± 1.50	K	NIST Webbook
tf	320.00 ± 1.00	K	NIST Webbook
tf	321.60 ± 0.10	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.36	J/mol×K	578.05	Joback Method

cpg	291.87	J/mol×K	611.92	Joback Method
cpg	301.73	J/mol×K	645.78	Joback Method
cpg	310.96	J/mol×K	679.65	Joback Method
cpg	319.60	J/mol×K	713.51	Joback Method
cpg	327.67	J/mol×K	747.38	Joback Method
cpg	335.20	J/mol×K	781.24	Joback Method
dvisc	0.0001082	Pa×s	578.05	Joback Method
dvisc	0.0023345	Pa×s	369.98	Joback Method
dvisc	0.0009851	Pa×s	411.59	Joback Method
dvisc	0.0068844	Pa×s	328.36	Joback Method
dvisc	0.0002711	Pa×s	494.82	Joback Method
dvisc	0.0001653	Pa×s	536.43	Joback Method
dvisc	0.0004871	Pa×s	453.20	Joback Method
hfust	15.61	kJ/mol	321.20	NIST Webbook
hfust	17.68	kJ/mol	321.20	NIST Webbook
hfust	17.68	kJ/mol	321.20	NIST Webbook
hfust	15.56	kJ/mol	321.60	NIST Webbook
hsubt	102.00 ± 0.70	kJ/mol	310.00	NIST Webbook
hvapt	67.00	kJ/mol	464.00	NIST Webbook
sfust	48.40	J/mol×K	321.60	NIST Webbook

Sources

Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids: https://www.doi.org/10.1021/je060078g

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C501520&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

hsub: Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume