

2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-

Other names:	Cinnamic acid, o-hydroxy-, (E)- o-Hydroxy-trans-cinnamic acid trans-o-Coumaric acid trans-o-Hydroxycinnamic acid trans-2-Hydroxycinnamic acid 2-Hydroxycinnamic acid, (E)- (E)-3-(2-Hydroxyphenyl)-2-propenoic acid ortho-Hydroxycinnamic acid, trans o-Coumaric acid, trans o-Hydroxycinnamic acid, trans 2-Hydroxycinnamic acid, trans (E)-2-Hydroxycinnamic acid (E)-o-Hydroxycinnamic acid 2-Propenoic acid, 3-(2-hydroxyphenyl)-, (2E)- NSC 32952
Inchi:	InChI=1S/C9H8O3/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6,10H,(H,11,12)/b6-5+
InchiKey:	PMOWTIHVNWZYFI-AATRIKPKSA-N
Formula:	C9H8O3
SMILES:	O=C(O)C=Cc1ccccc1O
Mol. weight [g/mol]:	164.16
CAS:	614-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-202.83	kJ/mol	Joback Method
hf	-317.46	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.490		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
tb	662.83	K	Joback Method
tc	884.22	K	Joback Method
tf	435.00	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.19	J/molxK	662.83	Joback Method
cpg	338.88	J/molxK	847.32	Joback Method
cpg	332.34	J/molxK	810.42	Joback Method
cpg	325.49	J/molxK	773.52	Joback Method
cpg	318.25	J/molxK	736.63	Joback Method
cpg	310.51	J/molxK	699.73	Joback Method
cpg	345.20	J/molxK	884.22	Joback Method
dvisc	0.0000077	Paxs	662.83	Joback Method
dvisc	0.0000130	Paxs	624.86	Joback Method
dvisc	0.0000232	Paxs	586.89	Joback Method
dvisc	0.0000452	Paxs	548.91	Joback Method
dvisc	0.0000971	Paxs	510.94	Joback Method
dvisc	0.0002358	Paxs	472.97	Joback Method
dvisc	0.0006684	Paxs	435.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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