

(E)-cinnamyl alcohol

Other names:

(E)-3-phenylprop-2-en-1-ol
2-Propen-1-ol, 3-phenyl-, (E)-
E-Cinnamic alcohol
trans-cinnamyl alcohol

Inchi:

InChI=1S/C9H10O/c10-8-4-7-9-5-2-1-3-6-9/h1-7,10H,8H2/b7-4+

InchiKey:

OCCDEMITAIZTP-QPJJXVBHSA-N

Formula:

C9H10O

SMILES:

OCC=Cc1ccccc1

Mol. weight [g/mol]:

134.18

CAS:

4407-36-7

Physical Properties

Property code	Value	Unit	Source
gf	80.71	kJ/mol	Joback Method
hf	-27.57	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.692		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
rinpol	1315.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1310.10		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1310.10		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1268.00		NIST Webbook

rinpol	1319.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2289.00		NIST Webbook
ripol	2284.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2334.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2334.00		NIST Webbook
tb	530.70	K	NIST Webbook
tc	732.08	K	Joback Method
tf	305.62	K	Determination and Correlation of Solubility and Thermodynamic Properties of trans-Cinnamyl Alcohol in Pure and Binary Solvents from 253.15 K to 293.15 K
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.22	J/mol×K	528.34	Joback Method
cpg	259.32	J/mol×K	562.30	Joback Method
cpg	269.69	J/mol×K	596.25	Joback Method
cpg	279.40	J/mol×K	630.21	Joback Method
cpg	288.47	J/mol×K	664.17	Joback Method
cpg	296.96	J/mol×K	698.12	Joback Method
cpg	304.90	J/mol×K	732.08	Joback Method
dvisc	0.0169277	Pa×s	273.35	Joback Method
dvisc	0.0040869	Pa×s	315.85	Joback Method
dvisc	0.0013823	Pa×s	358.35	Joback Method
dvisc	0.0005883	Pa×s	400.85	Joback Method
dvisc	0.0002950	Pa×s	443.34	Joback Method
dvisc	0.0001669	Pa×s	485.84	Joback Method
dvisc	0.0001035	Pa×s	528.34	Joback Method
hsubt	109.60	kJ/mol	297.50	NIST Webbook

Sources

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=C4407367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Correlation of Solubility and Thermodynamic Properties of trans-Cinnamyl Alcohol in Pure and Binary Solvents from 253.15 K to 293.15 K:	https://www.doi.org/10.1021/acs.jced.7b00665

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
hsubt:	Enthalpy of sublimation at a given temperature
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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