2-Propenoic acid, 3-phenyl-, ethyl ester

Other names:	Cinnamic acid, ethyl ester
	Ethyl 3-phenyl-2-propenoate
	Ethyl 3-phenylacrylate
	Ethyl 3-phenylpropenoate
	Ethyl benzylideneacetate
	Ethyl cinnamate
	Ethyl «beta»-phenylacrylate
	Ethyl Â«betaÂ»-phenylacrylate
	NSC 6773
	trans-Ethyl cinnamate
Inchi:	InChI=1S/C11H12O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-9H,2H2,1H3/b9-8+
InchiKey:	KBEBGUQPQBELIU-CMDGGOBGSA-N
Formula:	C11H12O2
SMILES:	CCOC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	176.21
CAS:	103-36-6

Physical Properties

Property code	Value	Unit	Source
gf	0.45	kJ/mol	Joback Method
hf	-161.42	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-3.00		Estimated Solubility Method
log10ws	-3.00		Aqueous Solubility Prediction Method
logp	2.263		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1433.10		NIST Webbook
rinpol	1435.50		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1447.00		NIST Webbook

rinpol	1464.00	NIST Webbook
rinpol	1446.00	NIST Webbook
rinpol	1460.00	NIST Webbook
rinpol	1431.00	NIST Webbook
rinpol	1426.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1462.00	NIST Webbook
rinpol	1436.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1463.00	NIST Webbook
rinpol	1460.00	NIST Webbook
rinpol	1474.00	NIST Webbook
rinpol	1426.00	NIST Webbook
rinpol	1431.00	NIST Webbook
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rinpol	1480.00	NIST Webbook
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ripol	2106.00	NIST Webbook
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ripol	2081.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2167.00		NIST Webbook
tb	544.20	K	NIST Webbook
tb	545.65 ± 0.50	K	NIST Webbook
tc	776.95	K	Joback Method
tf	307.23	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.27	J/mol×K	558.21	Joback Method
cpg	398.33	J/mol×K	776.95	Joback Method
cpg	388.43	J/mol×K	740.50	Joback Method
cpg	377.80	J/mol×K	704.04	Joback Method
cpg	366.41	J/mol×K	667.58	Joback Method

cpg	354.22	J/mol×K	631.12	Joback Method
cpg	341.18	J/mol×K	594.67	Joback Method
cpl	274.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0010842	Pa×s	349.06	Joback Method
dvisc	0.0001704	Pa×s	558.21	Joback Method
dvisc	0.0002188	Pa×s	516.38	Joback Method
dvisc	0.0002937	Pa×s	474.55	Joback Method
dvisc	0.0004172	Pa×s	432.72	Joback Method
dvisc	0.0006391	Pa×s	390.89	Joback Method
dvisc	0.0021241	Pa×s	307.23	Joback Method
hvapt	57.80	kJ/mol	498.50	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103366&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase 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
hvapt: Enthalpy of vaporization at a given temperature
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