2-Propenoic acid, 3-phenyl-, methyl ester, (E)-

Other names:	Cinnamic acid, methyl ester, (E)-
	(E)-Methyl cinnamate
	trans-Methyl cinnamate
	trans-Methyl 3-phenyl-2-propenoate
	Methyl (E)-cinnamate
	Methyl trans-cinnamate
	trans-Cinnamic acid methyl ester
	Methyl (E)-3-phenylprop-2-enoate
	Methyl (E)-3-phenylpropenoate
	Methyl cinnamate, (E)
	(E)-3-Phenylacrylic acid methyl ester
	Methyl (E)-3-phenyl-2-propenoate
	Methyl trans-3-phenyl-2-propenoate
Inchi:	InChI=1S/C10H10O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7+
InchiKey:	CCRCUPLGCSFEDV-BQYQJAHWSA-N
Formula:	C10H10O2
SMILES:	COC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	1754-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-7.97	kJ/mol	Joback Method
hf	-140.78	kJ/mol	Joback Method
hfus	18.69	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.873		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1379.00		NIST Webbook

rinpol	1380.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1376.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1364.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1364.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1381.00	NIST Webbook
rinpol	1381.00	NIST Webbook
rinpol	1392.40	NIST Webbook
rinpol	1352.00	NIST Webbook
rinpol	1398.00	NIST Webbook
rinpol	1375.00	NIST Webbook
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rinpol	1379.00	NIST Webbook
rinpol	1354.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	1379.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	2096.00	NIST Webbook
ripol	2050.00	NIST Webbook
ripol	2077.00	NIST Webbook
ripol	2074.00	NIST Webbook
ripol	2096.00	NIST Webbook

ripol	2046.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2047.00		NIST Webbook
tb	535.33	K	Joback Method
tc	757.99	K	Joback Method
tf	295.96	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.89	J/mol×K	535.33	Joback Method
cpg	294.93	J/mol×K	572.44	Joback Method
cpg	307.12	J/mol×K	609.55	Joback Method
cpg	318.52	J/mol×K	646.66	Joback Method
cpg	329.15	J/mol×K	683.77	Joback Method
cpg	339.04	J/mol×K	720.88	Joback Method
cpg	348.24	J/mol×K	757.99	Joback Method
dvisc	0.0021489	Pa×s	295.96	Joback Method
dvisc	0.0011171	Pa×s	335.86	Joback Method
dvisc	0.0006673	Pa×s	375.75	Joback Method
dvisc	0.0004400	Pa×s	415.65	Joback Method
dvisc	0.0003121	Pa×s	455.54	Joback Method
dvisc	0.0002340	Pa×s	495.44	Joback Method
dvisc	0.0001831	Pa×s	535.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1754627&Units=SI

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

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
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