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

Other names:	Cinnamic acid, methyl ester
	Methyl cinnamate
	Methyl cinnamylate
	Methyl 3-phenylpropenoate
	Methyl 3-phenyl-2-propenoate
	Methyl 3-phenylacrylate
	Methyl ester of cinnamic acid
	3-Phenyl-2-propenoic acid methyl ester
	Methyl 3-phenylprop-2-enoate
	NSC 9411
	SemaSORB 9815
	3-Phenyl-2-propenoic acid methyl ester (methyl cinnamate)
	Methyl cinnamate (isomer)
Inchi:	InChI=1S/C10H10O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-8H,1H3
InchiKey:	CCRCUPLGCSFEDV-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	COC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	103-26-4

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	1380.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1380.00		NIST Webbook

rinpol	1348.00	NIST Webbook
rinpol	1339.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1346.00	NIST Webbook
rinpol	1348.00	NIST Webbook
rinpol	1344.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1342.00	NIST Webbook
rinpol	1399.00	NIST Webbook
rinpol	1388.00	NIST Webbook
rinpol	1342.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1344.00	NIST Webbook
rinpol	1344.00	NIST Webbook
rinpol	1402.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1363.00	NIST Webbook
rinpol	1363.00	NIST Webbook
rinpol	1370.50	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1389.00	NIST Webbook
rinpol	1379.00	NIST Webbook
rinpol	1378.00	NIST Webbook
rinpol	1352.00	NIST Webbook
rinpol	1336.00	NIST Webbook
rinpol	1378.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1347.00	NIST Webbook
rinpol	1370.50	NIST Webbook
rinpol	1350.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1365.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1365.00	NIST Webbook
ripol	2040.00	NIST Webbook
ripol	2050.00	NIST Webbook
ripol	2103.00	NIST Webbook
ripol	2065.00	NIST Webbook
ripol	2020.00	NIST Webbook
ripol	2103.00	NIST Webbook

ripol	2062.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2051.00		NIST Webbook
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ripol	2050.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2071.00		NIST Webbook
ripol	2071.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2103.00		NIST Webbook
tb	534.20	K	NIST Webbook
tc	757.99	K	Joback Method
tf	308.00 ± 1.50	K	NIST Webbook
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.24	J/mol×K	757.99	Joback Method
cpg	329.15	J/mol×K	683.77	Joback Method
cpg	318.52	J/mol×K	646.66	Joback Method
cpg	307.12	J/mol×K	609.55	Joback Method

cpg	294.93	J/mol×K	572.44	Joback Method
cpg	281.89	J/mol×K	535.33	Joback Method
cpg	339.04	J/mol×K	720.88	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	0.0021489	Pa×s	295.96	Joback Method
dvisc	0.0001831	Pa×s	535.33	Joback Method
hfust	33.10	kJ/mol	309.00	NIST Webbook
hvapt	62.40	kJ/mol	310.50	NIST Webbook
hvapt	50.50 ± 0.50	kJ/mol	483.00	NIST Webbook
hvapt	53.80 ± 0.30	kJ/mol	483.00	NIST Webbook
hvapt	56.90 ± 0.20	kJ/mol	483.00	NIST Webbook
hvapt	59.90 ± 0.20	kJ/mol	483.00	NIST Webbook
hvapt	58.30	kJ/mol	443.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103264&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

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
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