2-Propenoic acid, 3-phenyl-, 1-methylethyl ester

Other names:	Cinnamic acid, isopropyl ester
	Isopropyl cinnamate
	Isopropylester kyseliny skoricove
	Isopropyl 3-phenylpropenoate
	1-Methylethyl 3-phenylpropenoate
	Isopropyl 3-phenyl-2-propenoate
Inchi:	InChI=1S/C12H14O2/c1-10(2)14-12(13)9-8-11-6-4-3-5-7-11/h3-10H,1-2H3/b9-8+
InchiKey:	RGACABDFLVLVCT-CMDGGOBGSA-N
Formula:	C12H14O2
SMILES:	CC(C)OC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	190.24
CAS:	7780-06-5

Physical Properties

Property code	Value	Unit	Source
gf	6.43	kJ/mol	Joback Method
hf	-187.34	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.651		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	580.65	K	Joback Method
tc	800.23	K	Joback Method
tf	303.50	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.76	J/mol×K	580.65	Joback Method
cpg	389.79	J/mol×K	617.25	Joback Method
cpg	403.87	J/mol×K	653.84	Joback Method
cpg	417.03	J/mol×K	690.44	Joback Method
cpg	429.31	J/mol×K	727.04	Joback Method
cpg	440.76	J/mol×K	763.63	Joback Method
cpg	451.41	J/mol×K	800.23	Joback Method
dvisc	0.0027204	Pa×s	303.50	Joback Method
dvisc	0.0012128	Pa×s	349.69	Joback Method
dvisc	0.0006529	Pa×s	395.88	Joback Method
dvisc	0.0004000	Pa×s	442.07	Joback Method
dvisc	0.0002689	Pa×s	488.27	Joback Method
dvisc	0.0001936	Pa×s	534.46	Joback Method
dvisc	0.0001469	Pa×s	580.65	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7780065&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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