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

Other names: Cinnamic acid, phenethyl ester
«beta»-Phenethyl cinnamate
«beta»-Phenylethyl cinnamate
Benzylcarbinyl cinnamate
Phenethyl cinnamate
Phenylethyl cinnamate
2-Phenylethyl cinnamate
2-Phenylethyl 3-phenyl-2-propenoate
Cinnamic acid, phenylethyl ester
NSC 16962

Inchi: InChI=1S/C17H16O2/c18-17(12-11-15-7-3-1-4-8-15)19-14-13-16-9-5-2-6-10-16/h1-12H,1

InchiKey: MJQVZIANGRDJBT-VAWYXSNFSA-N

Formula: C17H16O2

SMILES: O=C(C=Cc1ccccc1)OCCc1ccccc1

Mol. weight [g/mol]: 252.31

CAS: 103-53-7

Physical Properties

Property code	Value	Unit	Source
gf	163.38	kJ/mol	Joback Method
hf	-48.73	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.486		Crippen Method
mcvol	206.010	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2143.00		NIST Webbook
ripol	3100.00		NIST Webbook
tb	722.17	K	Joback Method
tc	959.64	K	Joback Method
tf	401.27	K	Joback Method

vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.46	J/mol×K	722.17	Joback Method
cpg	564.34	J/mol×K	761.75	Joback Method
cpg	578.95	J/mol×K	801.33	Joback Method
cpg	592.39	J/mol×K	840.90	Joback Method
cpg	604.74	J/mol×K	880.48	Joback Method
cpg	616.08	J/mol×K	920.06	Joback Method
cpg	626.50	J/mol×K	959.64	Joback Method
dvisc	0.0012341	Pa×s	401.27	Joback Method
dvisc	0.0006248	Pa×s	454.75	Joback Method
dvisc	0.0003650	Pa×s	508.24	Joback Method
dvisc	0.0002362	Pa×s	561.72	Joback Method
dvisc	0.0001649	Pa×s	615.20	Joback Method
dvisc	0.0001219	Pa×s	668.69	Joback Method
dvisc	0.0000943	Pa×s	722.17	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103537&Units=SI

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