Pentanoic acid, 3-phenyl-2-propenyl ester

Other names:	Cinnamyl N-valerate
	3-Phenyl-2-propenyl pentanoate
	Cinnamyl valerate
	Valeric acid, cinnamyl ester
Inchi:	InChI=1S/C14H18O2/c1-2-3-11-14(15)16-12-7-10-13-8-5-4-6-9-13/h4-10H,2-3,11-12H2,1
InchiKey:	FLSKWIBFXUNBAW-JXMROGBWSA-N
Formula:	C14H18O2
SMILES:	CCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	218.29
CAS:	10482-65-2

Physical Properties

Property code	Value	Unit	Source
gf	25.71	kJ/mol	Joback Method
hf	-223.34	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.433		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1705.00		NIST Webbook
ripol	2347.00		NIST Webbook
tb	626.85	K	Joback Method
tc	834.90	K	Joback Method
tf	341.04	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.32	J/mol×K	626.85	Joback Method
cpg	489.16	J/mol×K	661.52	Joback Method

cpg	504.05	J/mol×K	696.20	Joback Method
cpg	518.03	J/mol×K	730.87	Joback Method
cpg	531.13	J/mol×K	765.55	Joback Method
cpg	543.41	J/mol×K	800.22	Joback Method
cpg	554.89	J/mol×K	834.90	Joback Method
dvisc	0.0019011	Pa×s	341.04	Joback Method
dvisc	0.0009243	Pa×s	388.68	Joback Method
dvisc	0.0005261	Pa×s	436.31	Joback Method
dvisc	0.0003345	Pa×s	483.95	Joback Method
dvisc	0.0002307	Pa×s	531.58	Joback Method
dvisc	0.0001691	Pa×s	579.22	Joback Method
dvisc	0.0001300	Pa×s	626.85	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10482652&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
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