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

Other names: 2-methylbutyl cinnamate
Inchi: InChI=1S/C14H18O2/c1-3-12(2)11-16-14(15)10-9-13-7-5-4-6-8-13/h4-10,12H,3,11H2,1-2
InchiKey: SEGJDCGIQJESDC-MDZDMXLPSA-N
Formula: C14H18O2
SMILES: CCC(C)COC(=O)C=Cc1ccccc1
Mol. weight [g/mol]: 218.29
CAS: 4654-29-9

Physical Properties

Property code	Value	Unit	Source
gf	23.27	kJ/mol	Joback Method
hf	-228.62	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.289		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1717.60		NIST Webbook
tb	626.41	K	Joback Method
tc	838.56	K	Joback Method
tf	326.04	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.76	J/mol×K	626.41	Joback Method
cpg	489.96	J/mol×K	661.77	Joback Method
cpg	505.16	J/mol×K	697.13	Joback Method
cpg	519.40	J/mol×K	732.49	Joback Method
cpg	532.72	J/mol×K	767.84	Joback Method
cpg	545.17	J/mol×K	803.20	Joback Method
cpg	556.80	J/mol×K	838.56	Joback Method

dvisc	0.0024476	Pa×s	326.04	Joback Method
dvisc	0.0010623	Pa×s	376.10	Joback Method
dvisc	0.0005610	Pa×s	426.16	Joback Method
dvisc	0.0003388	Pa×s	476.23	Joback Method
dvisc	0.0002252	Pa×s	526.29	Joback Method
dvisc	0.0001607	Pa×s	576.35	Joback Method
dvisc	0.0001210	Pa×s	626.41	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=C4654299&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume