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

Other names: Cinnamic acid, isobutyl ester
Isobutyl cinnamate
Labdanol
Isobutyl cinammate

Inchi: InChI=1S/C13H16O2/c1-11(2)10-15-13(14)9-8-12-6-4-3-5-7-12/h3-9,11H,10H2,1-2H3/b9

InchiKey: IQZUZPKOFSOVET-CMDGGOBGSA-N

Formula: C13H16O2

SMILES: CC(C)COC(=O)C=Cc1ccccc1

Mol. weight [g/mol]: 204.26

CAS: 122-67-8

Physical Properties

Property code	Value	Unit	Source
gf	14.85	kJ/mol	Joback Method
hf	-207.98	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.899		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2230.00		NIST Webbook
ripol	2230.00		NIST Webbook
tb	603.53	K	Joback Method
tc	819.28	K	Joback Method
tf	314.77	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.50	J/mol×K	603.53	Joback Method
cpg	492.43	J/mol×K	783.32	Joback Method
cpg	480.44	J/mol×K	747.36	Joback Method
cpg	467.59	J/mol×K	711.40	Joback Method
cpg	453.85	J/mol×K	675.45	Joback Method
cpg	439.17	J/mol×K	639.49	Joback Method
cpg	503.60	J/mol×K	819.28	Joback Method
dvisc	0.0001338	Pa×s	603.53	Joback Method
dvisc	0.0001770	Pa×s	555.40	Joback Method
dvisc	0.0002470	Pa×s	507.28	Joback Method
dvisc	0.0003696	Pa×s	459.15	Joback Method
dvisc	0.0006078	Pa×s	411.02	Joback Method
dvisc	0.0011404	Pa×s	362.90	Joback Method
dvisc	0.0025937	Pa×s	314.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122678&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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