Propanoic acid, 2-methyl-, 3-phenylpropyl ester

Other names: Hydrocinnamyl isobutyrate
Isobutyric acid, 3-phenylpropyl ester
3-Phenylpropyl isobutyrate
Phenylpropyl iso-butyrate

Inchi: InChI=1S/C13H18O2/c1-11(2)13(14)15-10-6-9-12-7-4-3-5-8-12/h3-5,7-8,11H,6,9-10H2,1

InchiKey: VBTAKMZSMFMLGT-UHFFFAOYSA-N

Formula: C13H18O2

SMILES: CC(C)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 206.28

CAS: 103-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-65.37	kJ/mol	Joback Method
hf	-325.20	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	55.58	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.818		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	1996.00		NIST Webbook
tb	599.37	K	Joback Method
tc	806.35	K	Joback Method
tf	319.85	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.71	J/mol×K	599.37	Joback Method
cpg	459.89	J/mol×K	633.87	Joback Method

cpg	475.13	J/mol×K	668.36	Joback Method
cpg	489.48	J/mol×K	702.86	Joback Method
cpg	502.95	J/mol×K	737.36	Joback Method
cpg	515.57	J/mol×K	771.85	Joback Method
cpg	527.37	J/mol×K	806.35	Joback Method
dvisc	0.0027865	Pa×s	319.85	Joback Method
dvisc	0.0012714	Pa×s	366.44	Joback Method
dvisc	0.0006925	Pa×s	413.02	Joback Method
dvisc	0.0004266	Pa×s	459.61	Joback Method
dvisc	0.0002873	Pa×s	506.20	Joback Method
dvisc	0.0002068	Pa×s	552.78	Joback Method
dvisc	0.0001567	Pa×s	599.37	Joback Method

Sources

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=C103582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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