Benzenepropanoic acid, «beta»-methyl-, methyl ester

Other names:	Hydrocinnamic acid, «beta»-methyl-, methyl ester
	Methyl 3-phenylbutanoate
	Methyl 3-phenylbutyrate
	Methyl ester of «beta»-Methylbenzenepropanoic acid
	3-Phenylbutanoic acid methyl ester
Inchi:	InChI=1S/C11H14O2/c1-9(8-11(12)13-2)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	DSWKGCIHFICHAC-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	COC(=O)CC(C)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	3461-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-82.21	kJ/mol	Joback Method
hf	-283.92	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
ie	8.70 ± 0.20	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.353		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	553.61	K	Joback Method
tc	767.42	K	Joback Method
tf	297.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.73	J/mol×K	553.61	Joback Method
cpg	361.56	J/mol×K	589.25	Joback Method
cpg	375.53	J/mol×K	624.88	Joback Method

cpg	388.67	J/mol×K	660.52	Joback Method
cpg	401.00	J/mol×K	696.15	Joback Method
cpg	412.55	J/mol×K	731.79	Joback Method
cpg	423.32	J/mol×K	767.42	Joback Method
dvisc	0.0030377	Pa×s	297.31	Joback Method
dvisc	0.0014284	Pa×s	340.03	Joback Method
dvisc	0.0007949	Pa×s	382.74	Joback Method
dvisc	0.0004976	Pa×s	425.46	Joback Method
dvisc	0.0003393	Pa×s	468.18	Joback Method
dvisc	0.0002466	Pa×s	510.89	Joback Method
dvisc	0.0001883	Pa×s	553.61	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3461390&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume