2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester, (E)-

Other names: (E)-Methyl-p-methoxycinnamate
Methyl (E)-p-methoxycinnamate
p-Coumaric acid, methyl ether, methyl ester, trans-
p-Coumaric acid, methyl ether, methyl ester
Methyl (2E)-3-(4-methoxyphenyl)-2-propenoate

Inchi: InChI=1S/C11H12O3/c1-13-10-6-3-9(4-7-10)5-8-11(12)14-2/h3-8H,1-2H3/b8-5+

InchiKey: VEZIKIAGFYZTCI-VMPITWQZSA-N

Formula: C11H12O3

SMILES: COC(=O)C=Cc1ccc(OC)cc1

Mol. weight [g/mol]: 192.21

CAS: 3901-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-114.18	kJ/mol	Joback Method
hf	-305.11	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.881		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1768.10		NIST Webbook
tb	585.61	K	Joback Method
tc	802.77	K	Joback Method
tf	341.98	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.81	J/mol×K	585.61	Joback Method
cpg	364.16	J/mol×K	621.80	Joback Method
cpg	376.74	J/mol×K	658.00	Joback Method

cpg	388.57	J/mol×K	694.19	Joback Method
cpg	399.68	J/mol×K	730.38	Joback Method
cpg	410.06	J/mol×K	766.58	Joback Method
cpg	419.74	J/mol×K	802.77	Joback Method
dvisc	0.0012034	Pa×s	341.98	Joback Method
dvisc	0.0006894	Pa×s	382.59	Joback Method
dvisc	0.0004395	Pa×s	423.19	Joback Method
dvisc	0.0003032	Pa×s	463.80	Joback Method
dvisc	0.0002220	Pa×s	504.40	Joback Method
dvisc	0.0001703	Pa×s	545.00	Joback Method
dvisc	0.0001355	Pa×s	585.61	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3901073&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume