2-Propenal, 3-(3,4-dimethoxyphenyl)-

Other names:	Cinnamaldehyde, 3,4-dimethoxy-
	Coniferaldehyde methyl ether
	Methylconiferylaldehyde
	3,4-Dimethoxycinnamaldehyde
	Coniferyl aldehyde, methyl ether
	3-(3,4-dimethoxyphenyl)-2-propenal
Inchi:	InChI=1S/C11H12O3/c1-13-10-6-5-9(4-3-7-12)8-11(10)14-2/h3-8H,1-2H3/b4-3+
InchiKey:	KNUFNLWDGZQKKJ-ONEGZZNKSA-N
Formula:	C11H12O3
SMILES:	COc1ccc(C=CC=O)cc1OC
Mol. weight [g/mol]:	192.21
CAS:	4497-40-9

Physical Properties

Property code	Value	Unit	Source
gf	-94.41	kJ/mol	Joback Method
hf	-289.58	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.916		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1790.90		NIST Webbook
tb	585.38	K	Joback Method
tc	798.61	K	Joback Method
tf	346.57	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.06	J/mol×K	585.38	Joback Method

cpg	363.82	J/mol×K	620.92	Joback Method
cpg	375.91	J/mol×K	656.46	Joback Method
cpg	387.32	J/mol×K	692.00	Joback Method
cpg	398.07	J/mol×K	727.54	Joback Method
cpg	408.17	J/mol×K	763.07	Joback Method
cpg	417.63	J/mol×K	798.61	Joback Method
dvisc	0.0010663	Pa×s	346.57	Joback Method
dvisc	0.0006452	Pa×s	386.37	Joback Method
dvisc	0.0004288	Pa×s	426.17	Joback Method
dvisc	0.0003056	Pa×s	465.98	Joback Method
dvisc	0.0002297	Pa×s	505.78	Joback Method
dvisc	0.0001800	Pa×s	545.58	Joback Method
dvisc	0.0001458	Pa×s	585.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4497409&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