Ethanone, 1-(3,4-dimethoxyphenyl)-

Other names:	Acetophenone, 3',4'-dimethoxy-
	Acetoveratrone
	3,4-Dimethoxyphenyl methyl ketone
	3',4'-Dimethoxyacetophenone
	3,4-Dimethoxyacetophenone
	4'-Hydroxy-3'-methoxyacetophenone, methyl ether
	1-(3,4-Dimethoxyphenyl)ethanone
	1-(3,4-dimethoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O3/c1-7(11)8-4-5-9(12-2)10(6-8)13-3/h4-6H,1-3H3
InchiKey:	IQZLUWLMQNGTIW-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccc(C(C)=O)cc1OC
Mol. weight [g/mol]:	180.20
CAS:	1131-62-0

Physical Properties

Property code	Value	Unit	Source
gf	-212.45	kJ/mol	Joback Method
hf	-413.16	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.906		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1564.00		NIST Webbook
ripol	2393.00		NIST Webbook
ripol	2393.00		NIST Webbook
tb	560.20	K	NIST Webbook
tc	776.08	K	Joback Method
tf	348.31	K	Joback Method

vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.48	J/mol×K	563.55	Joback Method
cpg	336.25	J/mol×K	598.97	Joback Method
cpg	348.42	J/mol×K	634.39	Joback Method
cpg	359.98	J/mol×K	669.82	Joback Method
cpg	370.92	J/mol×K	705.24	Joback Method
cpg	381.23	J/mol×K	740.66	Joback Method
cpg	390.91	J/mol×K	776.08	Joback Method
dvisc	0.0010565	Pa×s	348.31	Joback Method
dvisc	0.0006746	Pa×s	384.18	Joback Method
dvisc	0.0004650	Pa×s	420.06	Joback Method
dvisc	0.0003399	Pa×s	455.93	Joback Method
dvisc	0.0002601	Pa×s	491.80	Joback Method
dvisc	0.0002064	Pa×s	527.68	Joback Method
dvisc	0.0001686	Pa×s	563.55	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131620&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume