Ethanone, 1-(2,5-dimethoxyphenyl)-

Other names: Acetophenone, 2',5'-dimethoxy-
2,5-Dimethoxyacetophenone
2',5'-Dimethoxyacetophenone
2-Acetyl-1,4-dimethoxybenzene
2,5-Dihydroxyacetophenone, dimethyl ether
1-(2,5-Dimethoxyphenyl)ethanone

Inchi: InChI=1S/C10H12O3/c1-7(11)9-6-8(12-2)4-5-10(9)13-3/h4-6H,1-3H3

InchiKey: FAXUIYJKGGUCBO-UHFFFAOYSA-N

Formula: C10H12O3

SMILES: COc1ccc(OC)c(C(C)=O)c1

Mol. weight [g/mol]: 180.20

CAS: 1201-38-3

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	1514.60		NIST Webbook
tb	563.55	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.70	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1201383&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume