2',6'-Dimethoxyacetophenone

Other names:	2,6-Dimethoxyacetophenone
	Ethanone, 1-(2,6-dimethoxyphenyl)-
	Acetophenone, 2',6'-dimethoxy-
	USAF K-2801
	2',6'-Dihydroxyacetophenone, dimethyl ether
	1-(2,6-Dimethoxyphenyl)ethanone
	1-(2,6-dimethoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O3/c1-7(11)10-8(12-2)5-4-6-9(10)13-3/h4-6H,1-3H3
InchiKey:	XEUGKOFTNAYMMX-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1cccc(OC)c1C(C)=O
Mol. weight [g/mol]:	180.20
CAS:	2040-04-2

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	1468.70		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1480.00		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	381.23	J/mol×K	740.66	Joback Method
cpg	370.92	J/mol×K	705.24	Joback Method
cpg	359.98	J/mol×K	669.82	Joback Method
cpg	348.42	J/mol×K	634.39	Joback Method
cpg	336.25	J/mol×K	598.97	Joback Method
cpg	390.91	J/mol×K	776.08	Joback Method
dvisc	0.0001686	Pa×s	563.55	Joback Method
dvisc	0.0002064	Pa×s	527.68	Joback Method
dvisc	0.0002601	Pa×s	491.80	Joback Method
dvisc	0.0003399	Pa×s	455.93	Joback Method
dvisc	0.0004650	Pa×s	420.06	Joback Method
dvisc	0.0006746	Pa×s	384.18	Joback Method
dvisc	0.0010565	Pa×s	348.31	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040042&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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