3,4-Dimethylbenzophenone

Other names:	Methanone, (3,4-dimethylphenyl)phenyl- Benzophenone, 3,4-dimethyl-
Inchi:	InChI=1S/C15H14O/c1-11-8-9-14(10-12(11)2)15(16)13-6-4-3-5-7-13/h3-10H,1-2H3
InchiKey:	JENOLWCGNVWTJN-UHFFFAOYSA-N
Formula:	C15H14O
SMILES:	Cc1ccc(C(=O)c2ccccc2)cc1C
Mol. weight [g/mol]:	210.27
CAS:	2571-39-3

Physical Properties

Property code	Value	Unit	Source
gf	152.06	kJ/mol	Joback Method
hf	-15.39	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hsub	107.90 ± 0.80	kJ/mol	NIST Webbook
hvap	61.61	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.534		Crippen Method
mcvol	176.260	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	659.79	K	Joback Method
tc	903.00	K	Joback Method
tf	386.62	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.31	J/mol×K	659.79	Joback Method
cpg	455.15	J/mol×K	700.33	Joback Method
cpg	469.79	J/mol×K	740.86	Joback Method
cpg	483.28	J/mol×K	781.40	Joback Method
cpg	495.70	J/mol×K	821.93	Joback Method
cpg	507.10	J/mol×K	862.47	Joback Method

cpg	517.55	J/mol×K	903.00	Joback Method
dvisc	0.0013483	Pa×s	386.62	Joback Method
dvisc	0.0007961	Pa×s	432.15	Joback Method
dvisc	0.0005197	Pa×s	477.68	Joback Method
dvisc	0.0003655	Pa×s	523.20	Joback Method
dvisc	0.0002719	Pa×s	568.73	Joback Method
dvisc	0.0002113	Pa×s	614.26	Joback Method
dvisc	0.0001701	Pa×s	659.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	613.20	K	99.20	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2571393&Units=SI

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
hsub: Enthalpy of sublimation 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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume