Ethanone, 1-(2,4-dimethylphenyl)-

Other names:	Acetophenone, 2',4'-dimethyl-
	2,4-Dimethylacetophenone
	2',4'-Dimethylacetophenone
	4-Acetyl-m-xylene
	(2,4-Dimethylphenyl)ethanone
	2,4-(CH3)2C6H3-COCH3
	1-(2,4-dimethylphenyl)ethanone
Inchi:	InChI=1S/C10H12O/c1-7-4-5-10(9(3)11)8(2)6-7/h4-6H,1-3H3
InchiKey:	HSDSKVWQTONQBJ-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CC(=O)c1ccc(C)cc1C
Mol. weight [g/mol]:	148.20
CAS:	89-74-7

Physical Properties

Property code	Value	Unit	Source
affp	882.60	kJ/mol	NIST Webbook
basg	850.80	kJ/mol	NIST Webbook
gf	-2.45	kJ/mol	Joback Method
hf	-148.72	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	48.20	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.506		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1221.40		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1221.40		NIST Webbook
rinpol	1233.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1861.00		NIST Webbook
tb	501.20	K	NIST Webbook
tc	735.99	K	Joback Method

tf	296.10 ± 0.70	K	NIST Webbook
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.59	J/mol×K	518.71	Joback Method
cpg	289.78	J/mol×K	554.92	Joback Method
cpg	302.26	J/mol×K	591.14	Joback Method
cpg	314.04	J/mol×K	627.35	Joback Method
cpg	325.13	J/mol×K	663.56	Joback Method
cpg	335.57	J/mol×K	699.77	Joback Method
cpg	345.38	J/mol×K	735.99	Joback Method
dvisc	0.0017002	Pa×s	303.85	Joback Method
dvisc	0.0010355	Pa×s	339.66	Joback Method
dvisc	0.0006932	Pa×s	375.47	Joback Method
dvisc	0.0004977	Pa×s	411.28	Joback Method
dvisc	0.0003768	Pa×s	447.09	Joback Method
dvisc	0.0002973	Pa×s	482.90	Joback Method
dvisc	0.0002423	Pa×s	518.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89747&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

affp:	Proton affinity
basg:	Gas basicity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume