

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

Other names:	3,4-Dimethylacetophenone 3',4'-Dimethylacetophenone (3,4-Dimethylphenyl)ethanone Acetophenone, 3',4'-dimethyl- 1-(3,4-Dimethylphenyl)ethanone 3,4-(CH ₃) ₂ C ₆ H ₃ -COCH ₃ 1-(3,4-dimethylphenyl)ethanone 1-(3,4-dimethylphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O/c1-7-4-5-10(9(3)11)6-8(7)2/h4-6H,1-3H3
InchiKey:	WPRAOXJIODQJR-UHFFFAOYSA-N
Formula:	C ₁₀ H ₁₂ O
SMILES:	<chem>CC(=O)c1ccc(C)c(C)c1</chem>
Mol. weight [g/mol]:	148.20
CAS:	3637-01-2

Physical Properties

Property code	Value	Unit	Source
affp	882.80	kJ/mol	NIST Webbook
basg	851.00	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
ripol	1831.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1823.00		NIST Webbook
tb	519.70	K	NIST Webbook
tb	516.20	K	NIST Webbook
tc	735.99	K	Joback Method

tf	268.10 ± 1.00	K	NIST Webbook
vc	0.493	m ³ /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	Paxs	303.85	Joback Method
dvisc	0.0010355	Paxs	339.66	Joback Method
dvisc	0.0006932	Paxs	375.47	Joback Method
dvisc	0.0004977	Paxs	411.28	Joback Method
dvisc	0.0003768	Paxs	447.09	Joback Method
dvisc	0.0002973	Paxs	482.90	Joback Method
dvisc	0.0002423	Paxs	518.71	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=C3637012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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