4-Acetylanisole

Other names:	1-(4-methoxyphenyl)ethanone
	4'-methoxyacetophenone
	4-Methoxyacetofenon
	4-Methoxyacetophenon
	4-Methoxyacetophenone
	4-Methoxyphenyl methyl ketone
	Acetanisole
	Acetophenone, 4'-methoxy-
	Acetophenone, p-methoxy-
	Anise ketone
	Ethanone, 1-(4-methoxyphenyl)-
	Linarodin
	Methyl 4-methoxyphenyl ketone
	Methyl p-methoxyphenyl ketone
	NSC 209523
	Novatone
	Vananote
	anisole, 4-acetyl-
	methyl (4-methoxyphenyl) ketone
	p-Methoxyacetophenone
	p-Methoxyphenyl methyl ketone
	p-Metoxyacetophenone
	p-acetylanisole
	para-Methoxyacetophenone
	para-Methoxyacetophenone (acetanisole)
Inchi:	InChI=1S/C9H10O2/c1-7(10)8-3-5-9(11-2)6-4-8/h3-6H,1-2H3
InchiKey:	NTPLXRHDUXRPNE-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	150.17
CAS:	100-06-1

Physical Properties

Property code	Value	Unit	Source
affp	895.60	kJ/mol	NIST Webbook
basg	863.70	kJ/mol	NIST Webbook

chl	-4669.80	kJ/mol	NIST Webbook
gf	-106.24	kJ/mol	Joback Method
hf	-248.83	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
ie	8.20 ± 0.10	eV	NIST Webbook
ie	8.62 ± 0.05	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.898		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1333.40		NIST Webbook
rinpol	1392.40		NIST Webbook
rinpol	1325.80		NIST Webbook
rinpol	1314.30		NIST Webbook
rinpol	1310.90		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1337.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2144.00		NIST Webbook

ripol	2120.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2164.00		NIST Webbook
ripol	2116.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	531.20	K	NIST Webbook
tc	730.64	K	Joback Method
tf	311.40 ± 0.70	K	NIST Webbook
tf	311.65 ± 1.50	K	NIST Webbook
tf	312.00 ± 3.00	K	NIST Webbook
tf	311.15 ± 1.00	K	NIST Webbook
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.07	J/mol×K	585.73	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	291.03	J/mol×K	621.95	Joback Method
cpg	256.24	J/mol×K	513.27	Joback Method
cpg	268.48	J/mol×K	549.50	Joback Method
dvisc	0.0010297	Pa×s	337.45	Joback Method
dvisc	0.0006754	Pa×s	372.62	Joback Method
dvisc	0.0004764	Pa×s	407.78	Joback Method
dvisc	0.0003552	Pa×s	442.94	Joback Method
dvisc	0.0002765	Pa×s	478.11	Joback Method
dvisc	0.0017319	Pa×s	302.29	Joback Method
dvisc	0.0002227	Pa×s	513.27	Joback Method
hsubt	93.70	kJ/mol	308.00	NIST Webbook
hsubt	77.70	kJ/mol	288.00	NIST Webbook
hsubt	77.70 ± 0.20	kJ/mol	311.40	NIST Webbook
hvapt	66.50	kJ/mol	322.50	NIST Webbook
hvapt	87.80	kJ/mol	298.15	Standard molar enthalpy of formation of methoxyacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	3.50	NIST Webbook
tbrp	411.70	K	2.00	NIST Webbook

Sources

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=C100061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard molar enthalpy of formation of methoxyacetophenone isomers:	https://www.doi.org/10.1016/j.jct.2014.03.027

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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