ortho-Methoxyacetophenone

Other names:	1-(2-methoxyphenyl)ethan-1-one 2'-methoxyacetophenone 2-Methoxyacetophenone 2-Methoxyacetylbenzene 2-acetylanisole Acetophenone, 2'-methoxy- Ethanone, 1-(2-methoxyphenyl)- methyl (2-methoxyphenyl) ketone o-Acetanisole o-Acetylanisole o-Methoxyacetophenone
Inchi:	InChI=1S/C9H10O2/c1-7(10)8-5-3-4-6-9(8)11-2/h3-6H,1-2H3
InchiKey:	DWPLEOPKBWNPQV-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COc1ccccc1C(C)=O
Mol. weight [g/mol]:	150.17
CAS:	579-74-8

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-2.25		Crippen Method
logp	1.898		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1285.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1975.00		NIST Webbook

tb	513.27	K	Joback Method
tc	730.64	K	Joback Method
tf	302.29	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.24	J/mol×K	513.27	Joback Method
cpg	268.48	J/mol×K	549.50	Joback Method
cpg	280.07	J/mol×K	585.73	Joback Method
cpg	291.03	J/mol×K	621.95	Joback Method
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
dvisc	0.0017319	Pa×s	302.29	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	0.0002227	Pa×s	513.27	Joback Method
hvapt	66.70	kJ/mol	298.15	Standard molar enthalpy of formation of methoxyacetophenone isomers

Sources

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
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=C579748&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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume