3-Buten-2-one, 4-(4-methoxyphenyl)-

Other names:	3-Buten-2-one, 4-(p-methoxyphenyl)-
	p-Anisilidenacetone
	p-Methoxybenzalacetone
	p-Methoxybenzylideneacetone
	Methyl p-methoxystyryl ketone
	4-Methoxybenzylideneacetone
	4-(4-Methoxyphenyl)-3-buten-2-one
	1-(p-Methoxyphenyl)-1-buten-3-one
	4'-Methoxybenzylideneacetone
	4-Methoxybenzalacetone
	Anisalacetone
	p-Anisalacetone
	1-(4-Methoxyphenyl)-but-1-en-3-one
	4-(p-Methoxyphenyl)-3-buten-2-one
	4-Methoxystyryl methyl ketone
	NSC 31752
	NSC 7946
	p-Methoxystyryl methyl ketone
Inchi:	InChI=1S/C11H12O2/c1-9(12)3-4-10-5-7-11(13-2)8-6-10/h3-8H,1-2H3/b4-3+
InchiKey:	WRRZKDVBPZBNJN-ONEGZZNKSA-N
Formula:	C11H12O2
SMILES:	COc1ccc(C=CC(C)=O)cc1
Mol. weight [g/mol]:	176.21
CAS:	943-88-4

Physical Properties

Property code	Value	Unit	Source
chs	-5763.50	kJ/mol	NIST Webbook
gf	-9.18	kJ/mol	Joback Method
hf	-172.89	kJ/mol	Joback Method
hfs	-309.00	kJ/mol	NIST Webbook
hfus	20.89	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.297		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method

tb	563.19	K	Joback Method
tc	783.00	K	Joback Method
tf	319.75	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.84	J/mol×K	563.19	Joback Method
cpg	340.44	J/mol×K	599.82	Joback Method
cpg	353.23	J/mol×K	636.46	Joback Method
cpg	365.23	J/mol×K	673.09	Joback Method
cpg	376.46	J/mol×K	709.73	Joback Method
cpg	386.97	J/mol×K	746.36	Joback Method
cpg	396.77	J/mol×K	783.00	Joback Method
dvisc	0.0015957	Pa×s	319.75	Joback Method
dvisc	0.0008853	Pa×s	360.32	Joback Method
dvisc	0.0005534	Pa×s	400.90	Joback Method
dvisc	0.0003771	Pa×s	441.47	Joback Method
dvisc	0.0002741	Pa×s	482.04	Joback Method
dvisc	0.0002094	Pa×s	522.62	Joback Method
dvisc	0.0001663	Pa×s	563.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C943884&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

chs: Standard solid 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
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume