Ethanone, 2-bromo-1-(4-methoxyphenyl)-

Other names:	Acetophenone, 2-bromo-4'-methoxy- «alpha»-Bromo-p-methoxyacetophenone «alpha»-Bromo-4-methoxyacetophenone «omega»-Bromo-p-methoxyacetophenone «omega»-Bromo-4-methoxyacetophenone 2-Bromo-p-methoxyacetophenone 2-Bromo-4'-methoxyacetophenone 2-Bromo-1-(4-methoxyphenyl)-1-ethanone Bromomethyl p-anisyl ketone 4'-Methoxy-2-bromoacetophenone p-Methoxyphenacyl bromide 4-Methoxyphenacyl bromide 4'-Methoxyphenacyl bromide 2-(4-Methoxyphenyl)-2-oxoethyl bromide «alpha»-Bromo-4'-methoxyacetophenone «omega»-Bromo-4'-methoxyacetophenone 2-Bromo-1-(4-methoxyphenyl)ethanone Bromomethyl 4-methoxyphenyl ketone
Inchi:	InChI=1S/C9H9BrO2/c1-12-8-4-2-7(3-5-8)9(11)6-10/h2-5H,6H2,1H3
InchiKey:	XQJAHBHCLXUGEP-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	COc1ccc(C(=O)CBr)cc1
Mol. weight [g/mol]:	229.07
CAS:	2632-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-222.50	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.273		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method

tb	579.43	K	Joback Method
tc	811.07	K	Joback Method
tf	362.09	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/mol×K	579.43	Joback Method
cpg	302.44	J/mol×K	618.04	Joback Method
cpg	313.06	J/mol×K	656.64	Joback Method
cpg	322.96	J/mol×K	695.25	Joback Method
cpg	332.17	J/mol×K	733.85	Joback Method
cpg	340.71	J/mol×K	772.46	Joback Method
cpg	348.60	J/mol×K	811.07	Joback Method
dvisc	0.0015157	Pa×s	362.09	Joback Method
dvisc	0.0009661	Pa×s	398.31	Joback Method
dvisc	0.0006638	Pa×s	434.54	Joback Method
dvisc	0.0004832	Pa×s	470.76	Joback Method
dvisc	0.0003681	Pa×s	506.98	Joback Method
dvisc	0.0002908	Pa×s	543.21	Joback Method
dvisc	0.0002365	Pa×s	579.43	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2632135&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy
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