2-BROMO-2'-METHOXYACETOPHENONE

Other names:	2-Methoxyphenacyl bromide
	Ethanone, 2-bromo-1-(2-methoxyphenyl)-
	bromomethyl 2-methoxyphenyl ketone
	o-Methoxy phenacylbromide
	«alpha»-Bromo-o-methoxyacetophenone
Inchi:	InChI=1S/C9H9BrO2/c1-12-9-5-3-2-4-7(9)8(11)6-10/h2-5H,6H2,1H3
InchiKey:	GKNCPTLOPRDYMH-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	COc1ccccc1C(=O)CBr
Mol. weight [g/mol]:	229.07

Physical Properties

Property code	Value	Unit	Source
hf	-233.95	kJ/mol	Cheméo Relay (1.0)
hfus	20.79	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
logp	2.273		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	561.69	K	Cheméo Relay (1.0)
tf	346.01	K	Cheméo Relay (1.0)

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=C31949210&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tf:	Normal melting (fusion) point