2-BROMO-3'-METHOXYACETOPHENONE

Other names:	m-Methoxyphenacyl bromide
	3-Methoxyphenacyl bromide
	Ethanone, 2-bromo-1-(3-methoxyphenyl)-
	bromomethyl 3-methoxyphenyl ketone
Inchi:	InChI=1S/C9H9BrO2/c1-12-8-4-2-3-7(5-8)9(11)6-10/h2-5H,6H2,1H3
InchiKey:	IOOHBIFQNQQUFI-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	COc1cccc(C(=O)CBr)c1
Mol. weight [g/mol]:	229.07

Physical Properties

Property code	Value	Unit	Source
hf	-229.72	kJ/mol	Cheméo Relay (1.0)
hfus	20.79	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-3.00		Cheméo Relay (1.0)
logp	2.273		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	565.79	K	Cheméo Relay (1.0)
tc	777.48	K	Cheméo Relay (1.0)
tf	334.37	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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5000657&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):

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
tc: Critical Temperature
tf: Normal melting (fusion) point