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

Other names:	Acetophenone, 2-bromo-4'-methyl-
	«alpha»-Bromo-p-methylacetophenone
	«alpha»-Bromo-4-methylacetophenone
	«omega»-Bromo-p-methylacetophenone
	2-Bromo-p-methylacetophenone
	2-Bromo-4'-methylacetophenone
	p-Methyl-«alpha»-bromoacetophenone
	p-Methyl-«omega»-bromoacetophenone
	p-Methylphenacyl bromide
	4-Methylphenacyl bromide
Inchi:	InChI=1S/C9H9BrO/c1-7-2-4-8(5-3-7)9(11)6-10/h2-5H,6H2,1H3
InchiKey:	KRVGXFREOJHJAX-UHFFFAOYSA-N
Formula:	C9H9BrO
SMILES:	Cc1ccc(C(=O)CBr)cc1
Mol. weight [g/mol]:	213.07
CAS:	619-41-0

Physical Properties

Property code	Value	Unit	Source
gf	13.08	kJ/mol	Joback Method
hf	-90.28	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	51.75	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.573		Crippen Method
mcvol	132.980	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	557.01	K	Joback Method
tc	791.91	K	Joback Method
tf	339.86	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.87	J/mol×K	557.01	Joback Method
cpg	280.43	J/mol×K	596.16	Joback Method
cpg	291.18	J/mol×K	635.31	Joback Method
cpg	301.16	J/mol×K	674.46	Joback Method
cpg	310.41	J/mol×K	713.61	Joback Method
cpg	318.99	J/mol×K	752.76	Joback Method
cpg	326.92	J/mol×K	791.91	Joback Method
dvisc	0.0020020	Pa×s	339.86	Joback Method
dvisc	0.0012473	Pa×s	376.05	Joback Method
dvisc	0.0008444	Pa×s	412.24	Joback Method
dvisc	0.0006088	Pa×s	448.44	Joback Method
dvisc	0.0004609	Pa×s	484.63	Joback Method
dvisc	0.0003627	Pa×s	520.82	Joback Method
dvisc	0.0002945	Pa×s	557.01	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619410&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

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
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