1-Propanone, 2-bromo-1-phenyl-

Other names:	1-Benzoyl-1-bromoethane
	«alpha»-Bromoethyl phenyl ketone
	1-Bromoethyl phenyl ketone
	«alpha»-Bromopropiophenone
	2-Bromopropiophenone
	«alpha»-Methylphenacyl bromide
	Propiophenone, 2-bromo-
	alpha-Bromopropiophenone
	TL 336
	NSC 89689
Inchi:	InChI=1S/C9H9BrO/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	WPDWOCRJBPXJFM-UHFFFAOYSA-N
Formula:	C9H9BrO
SMILES:	CC(Br)C(=O)c1ccccc1
Mol. weight [g/mol]:	213.07
CAS:	2114-00-3

Physical Properties

Property code	Value	Unit	Source
gf	20.27	kJ/mol	Joback Method
hf	-84.09	kJ/mol	Joback Method
hfus	16.47	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.653		Crippen Method
mcvol	132.980	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	520.70	K	NIST Webbook
tc	790.80	K	Joback Method
tf	312.34	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.02	J/mol×K	551.59	Joback Method
cpg	322.45	J/mol×K	750.94	Joback Method
cpg	313.61	J/mol×K	711.07	Joback Method
cpg	304.01	J/mol×K	671.20	Joback Method
cpg	293.58	J/mol×K	631.33	Joback Method
cpg	282.27	J/mol×K	591.46	Joback Method
cpg	330.58	J/mol×K	790.80	Joback Method
dvisc	0.0002837	Pa×s	551.59	Joback Method
dvisc	0.0003638	Pa×s	511.72	Joback Method
dvisc	0.0004866	Pa×s	471.84	Joback Method
dvisc	0.0006866	Pa×s	431.97	Joback Method
dvisc	0.0010391	Pa×s	392.09	Joback Method
dvisc	0.0017274	Pa×s	352.22	Joback Method
dvisc	0.0032693	Pa×s	312.34	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2114003&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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