Ethanone, 2-bromo-1-phenyl-

Other names: .alpha.-bromoacetophenone
1-Phenyl-2-bromoethanone
2-Bromo-1-phenylethanone
2-bromoacetophenone
Acetophenone, 2-bromo-
Benzoylmethyl bromide
Bromoacetophenone
Bromomethyl phenyl ketone
NSC 9807
Stauffer 4644
UN 2645
phenacyl bromide
«alpha»-Bromoacetophenone
«omega»-Bromacetophenone
«omega»-Bromoacetophenone

Inchi: InChI=1S/C8H7BrO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H,6H2

InchiKey: LIGACIXOYTUXAW-UHFFFAOYSA-N

Formula: C8H7BrO

SMILES: O=C(CBr)c1ccccc1

Mol. weight [g/mol]: 199.04

CAS: 70-11-1

Physical Properties

Property code	Value	Unit	Source
gf	14.29	kJ/mol	Joback Method
hf	-58.17	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.264		Crippen Method
mcvol	118.890	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1304.00		NIST Webbook
ripol	1971.00		NIST Webbook
tb	529.15	K	Joback Method

tc	767.60	K	Joback Method
tf	324.00 ± 1.00	K	NIST Webbook
tf	324.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.33	J/mol×K	529.15	Joback Method
cpg	237.17	J/mol×K	568.89	Joback Method
cpg	247.18	J/mol×K	608.63	Joback Method
cpg	256.40	J/mol×K	648.37	Joback Method
cpg	264.89	J/mol×K	688.12	Joback Method
cpg	272.68	J/mol×K	727.86	Joback Method
cpg	279.84	J/mol×K	767.60	Joback Method
dvisc	0.0026258	Pa×s	316.07	Joback Method
dvisc	0.0015606	Pa×s	351.58	Joback Method
dvisc	0.0010205	Pa×s	387.10	Joback Method
dvisc	0.0007166	Pa×s	422.61	Joback Method
dvisc	0.0005316	Pa×s	458.12	Joback Method
dvisc	0.0004117	Pa×s	493.64	Joback Method
dvisc	0.0003299	Pa×s	529.15	Joback Method
hvapt	90.90	kJ/mol	298.15	Calorimetric study of bromoacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	2.40	NIST Webbook
tbrp	408.00	K	2.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70111&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calorimetric study of bromoacetophenone isomers:	https://www.doi.org/10.1016/j.jct.2014.06.028
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume