Bromoacetone

Other names:	2-Propanone, 1-bromo-
	«alpha»-Bromoacetone
	Acetonyl bromide
	Acetylmethyl bromide
	1-Bromo-2-propanone
	CH3COCH2Br
	2-Propanone, bromo-
	Bromomethyl methyl ketone
	Bromo-2-propanone
	B-Stoff
	Martonite
	Monobromoacetone
	Rcra waste number P017
	UN 1569
	1-Bromoacetone
	«alpha»-Bromopropanone
Inchi:	InChI=1S/C3H5BrO/c1-3(5)2-4/h2H2,1H3
InchiKey:	VQFAIAKCILWQPZ-UHFFFAOYSA-N
Formula:	C3H5BrO
SMILES:	CC(=O)CBr
Mol. weight [g/mol]:	136.97
CAS:	598-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-140.22	kJ/mol	Joback Method
hf	-180.00 ± 8.40	kJ/mol	NIST Webbook
hfus	10.41	kJ/mol	Joback Method
hvap	35.45	kJ/mol	Joback Method
ie	9.73	eV	NIST Webbook
log10ws	-0.79		Crippen Method
logp	0.970		Crippen Method
mcvol	72.200	ml/mol	McGowan Method
pc	5296.96	kPa	Joback Method
rinpol	751.00		NIST Webbook
ripol	1030.00		NIST Webbook
tb	388.07	K	Joback Method

tc	589.55	K	Joback Method
tf	233.30	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.72	J/mol×K	388.07	Joback Method
cpg	111.35	J/mol×K	421.65	Joback Method
cpg	116.70	J/mol×K	455.23	Joback Method
cpg	121.76	J/mol×K	488.81	Joback Method
cpg	126.56	J/mol×K	522.39	Joback Method
cpg	131.10	J/mol×K	555.97	Joback Method
cpg	135.39	J/mol×K	589.55	Joback Method
dvisc	0.0031172	Pa×s	233.30	Joback Method
dvisc	0.0019296	Pa×s	259.10	Joback Method
dvisc	0.0013029	Pa×s	284.89	Joback Method
dvisc	0.0009390	Pa×s	310.69	Joback Method
dvisc	0.0007116	Pa×s	336.48	Joback Method
dvisc	0.0005609	Pa×s	362.27	Joback Method
dvisc	0.0004564	Pa×s	388.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	409.70	K	96.70	NIST Webbook

Sources

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=C598312&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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