2-Butanone, 1-bromo-3,3-dimethyl-

Other names:	1-Bromo-3,3-dimethyl-2-butanone
	Bromomethyl tert-butyl ketone
	1-Bromopinacolin
	Bromopinacolone
	«alpha»-Bromopinacolone
	1-Bromopinacolone
	tert-Butyl Bromomethyl ketone
	3,3-Dimethyl-2-oxobutyl bromide
	Pivaloylmethyl bromide
	1-Bromo-3,3-dimethylbutan-2-one
	Bromopinacolin
	NSC 25307
Inchi:	InChI=1S/C6H11BrO/c1-6(2,3)5(8)4-7/h4H2,1-3H3
InchiKey:	SAIRZMWXVJEBMO-UHFFFAOYSA-N
Formula:	C6H11BrO
SMILES:	CC(C)(C)C(=O)CBr
Mol. weight [g/mol]:	179.06
CAS:	5469-26-1

Physical Properties

Property code	Value	Unit	Source
gf	-112.12	kJ/mol	Joback Method
hf	-262.17	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	40.84	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.997		Crippen Method
mcvol	114.470	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	453.48	K	Joback Method
tc	662.19	K	Joback Method
tf	269.53	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.68	J/mol×K	453.48	Joback Method
cpg	227.74	J/mol×K	488.26	Joback Method
cpg	238.09	J/mol×K	523.05	Joback Method
cpg	247.75	J/mol×K	557.83	Joback Method
cpg	256.78	J/mol×K	592.62	Joback Method
cpg	265.21	J/mol×K	627.40	Joback Method
cpg	273.08	J/mol×K	662.19	Joback Method
dvisc	0.0047911	Pa×s	269.53	Joback Method
dvisc	0.0025669	Pa×s	300.19	Joback Method
dvisc	0.0015439	Pa×s	330.85	Joback Method
dvisc	0.0010122	Pa×s	361.50	Joback Method
dvisc	0.0007089	Pa×s	392.16	Joback Method
dvisc	0.0005228	Pa×s	422.82	Joback Method
dvisc	0.0004018	Pa×s	453.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.00	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5469261&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume