2-Butanone, 3-bromo-

Other names: 3-Bromo-2-butanone
3-bromobutan-2-one
Inchi: InChI=1S/C4H7BrO/c1-3(5)4(2)6/h3H,1-2H3
InchiKey: BNBOUFHCTIFWHN-UHFFFAOYSA-N
Formula: C4H7BrO
SMILES: CC(=O)C(C)Br
Mol. weight [g/mol]: 151.00
CAS: 814-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-134.24	kJ/mol	Joback Method
hf	-217.42	kJ/mol	Joback Method
hfus	9.48	kJ/mol	Joback Method
hvap	37.29	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.359		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	410.51	K	Joback Method
tc	615.14	K	Joback Method
tf	229.57	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.44	J/mol×K	410.51	Joback Method
cpg	146.94	J/mol×K	444.61	Joback Method
cpg	154.04	J/mol×K	478.72	Joback Method
cpg	160.77	J/mol×K	512.82	Joback Method
cpg	167.14	J/mol×K	546.93	Joback Method
cpg	173.16	J/mol×K	581.03	Joback Method
cpg	178.84	J/mol×K	615.14	Joback Method

dvisc	0.0047331	Pa×s	229.57	Joback Method
dvisc	0.0025078	Pa×s	259.73	Joback Method
dvisc	0.0015165	Pa×s	289.88	Joback Method
dvisc	0.0010082	Pa×s	320.04	Joback Method
dvisc	0.0007191	Pa×s	350.20	Joback Method
dvisc	0.0005411	Pa×s	380.35	Joback Method
dvisc	0.0004246	Pa×s	410.51	Joback Method
hvapt	46.40	kJ/mol	357.50	NIST Webbook

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=C814755&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
hvapt: Enthalpy of vaporization at a given temperature
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.