

2-Butanone, 1-bromo-

Other names:	1-Bromo-2-butanone Bromomethyl ethyl ketone TL 819 1-bromobutanone
Inchi:	InChI=1S/C4H7BrO/c1-2-4(6)3-5/h2-3H2,1H3
InchiKey:	CCXQVBSQUQCEE-UHFFFAOYSA-N
Formula:	C4H7BrO
SMILES:	CCC(=O)CBr
Mol. weight [g/mol]:	151.00
CAS:	816-40-0

Physical Properties

Property code	Value	Unit	Source
gf	-131.80	kJ/mol	Joback Method
hf	-212.14	kJ/mol	Joback Method
hfus	13.00	kJ/mol	Joback Method
hvap	37.68	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.360		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
tb	410.95	K	Joback Method
tc	610.68	K	Joback Method
tf	244.57	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.96	J/molxK	577.39	Joback Method
cpg	166.11	J/molxK	544.10	Joback Method
cpg	159.95	J/molxK	510.82	Joback Method
cpg	153.44	J/molxK	477.53	Joback Method
cpg	146.58	J/molxK	444.24	Joback Method

cpg	139.36	J/molxK	410.95	Joback Method
cpg	177.49	J/molxK	610.68	Joback Method
dvisc	0.0033149	Paxs	244.57	Joback Method
dvisc	0.0004413	Paxs	410.95	Joback Method
dvisc	0.0005469	Paxs	383.22	Joback Method
dvisc	0.0007008	Paxs	355.49	Joback Method
dvisc	0.0009365	Paxs	327.76	Joback Method
dvisc	0.0013202	Paxs	300.03	Joback Method
dvisc	0.0019962	Paxs	272.30	Joback Method
hvapt	49.90	kJ/mol	375.00	NIST Webbook
hvapt	47.70	kJ/mol	349.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	20.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C816400&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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