

1-Bromo-3-methylbutan-2-one

Inchi:	InChI=1S/C5H9BrO/c1-4(2)5(7)3-6/h4H,3H2,1-2H3
InchiKey:	NNTPEAXKKUPBHQ-UHFFFAOYSA-N
Formula:	C5H9BrO
SMILES:	CC(C)C(=O)CBr
Mol. weight [g/mol]:	165.03

Physical Properties

Property code	Value	Unit	Source
gf	-125.82	kJ/mol	Joback Method
hf	-238.06	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	39.52	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.606		Crippen Method
mcvol	100.380	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpola	930.00		NIST Webbook
rinpola	930.00		NIST Webbook
tb	433.39	K	Joback Method
tc	635.84	K	Joback Method
tf	240.84	K	Joback Method
vc	0.378	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.53	J/molxK	433.39	Joback Method
cpg	184.48	J/molxK	467.13	Joback Method
cpg	192.98	J/molxK	500.87	Joback Method
cpg	201.03	J/molxK	534.61	Joback Method
cpg	208.66	J/molxK	568.36	Joback Method
cpg	215.87	J/molxK	602.10	Joback Method
cpg	222.70	J/molxK	635.84	Joback Method
dvisc	0.0048520	Paxs	240.84	Joback Method

dvisc	0.0025100	Paxs	272.93	Joback Method
dvisc	0.0014916	Paxs	305.02	Joback Method
dvisc	0.0009788	Paxs	337.12	Joback Method
dvisc	0.0006910	Paxs	369.21	Joback Method
dvisc	0.0005158	Paxs	401.30	Joback Method
dvisc	0.0004021	Paxs	433.39	Joback Method

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=R412781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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