

Butane, 2-bromo-1-methoxy

Inchi:	InChI=1S/C5H11BrO/c1-3-5(6)4-7-2/h5H,3-4H2,1-2H3
InchiKey:	MPXVTXBMYIRQGB-UHFFFAOYSA-N
Formula:	C5H11BrO
SMILES:	CCC(Br)COC
Mol. weight [g/mol]:	167.04

Physical Properties

Property code	Value	Unit	Source
gf	-101.90	kJ/mol	Joback Method
hf	-257.70	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	35.18	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.806		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	844.00		NIST Webbook
tb	401.94	K	Joback Method
tc	591.17	K	Joback Method
tf	213.14	K	Joback Method
vc	0.390	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.68	J/molxK	401.94	Joback Method
cpg	192.05	J/molxK	433.48	Joback Method
cpg	201.06	J/molxK	465.02	Joback Method
cpg	209.73	J/molxK	496.55	Joback Method
cpg	218.06	J/molxK	528.09	Joback Method
cpg	226.05	J/molxK	559.63	Joback Method
cpg	233.72	J/molxK	591.17	Joback Method
dvisc	0.0044942	Paxs	213.14	Joback Method
dvisc	0.0021444	Paxs	244.61	Joback Method

dvisc	0.0012112	Paxs	276.07	Joback Method
dvisc	0.0007689	Paxs	307.54	Joback Method
dvisc	0.0005311	Paxs	339.01	Joback Method
dvisc	0.0003907	Paxs	370.47	Joback Method
dvisc	0.0003015	Paxs	401.94	Joback Method

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=R11997&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
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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