

Butane, 2-methoxy-3-methyl-

Inchi:	InChI=1S/C6H14O/c1-5(2)6(3)7-4/h5-6H,1-4H3
InchiKey:	JPUDLQKLSRSGN-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	COC(C)C(C)C
Mol. weight [g/mol]:	102.17
CAS:	62016-49-3

Physical Properties

Property code	Value	Unit	Source
gf	-110.24	kJ/mol	Joback Method
hf	-309.95	kJ/mol	Joback Method
hfus	5.44	kJ/mol	Joback Method
hvap	30.58	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.677		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	358.22	K	Joback Method
tc	530.65	K	Joback Method
tf	149.61	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.53	J/molxK	358.22	Joback Method
cpg	232.49	J/molxK	501.91	Joback Method
cpg	222.93	J/molxK	473.18	Joback Method
cpg	213.06	J/molxK	444.44	Joback Method
cpg	202.86	J/molxK	415.70	Joback Method
cpg	192.36	J/molxK	386.96	Joback Method
cpg	241.73	J/molxK	530.65	Joback Method
dvisc	0.0002102	Paxs	358.22	Joback Method
dvisc	0.0002900	Paxs	323.45	Joback Method

dvisc	0.0004325	Paxs	288.68	Joback Method
dvisc	0.0007195	Paxs	253.92	Joback Method
dvisc	0.0014068	Paxs	219.15	Joback Method
dvisc	0.0035421	Paxs	184.38	Joback Method
dvisc	0.0136988	Paxs	149.61	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=C62016493&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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