Butane, 1-methoxy-3-methyl-

Other names:	Ether, isopentyl methyl
	Isopentyl methyl ether
	(CH3)2CHCH2CH2OCH3
	4-Methoxy-2-methylbutane
	1-Methoxy-isopentane
	Methyl isopentyl ether
Inchi:	InChI=1S/C6H14O/c1-6(2)4-5-7-3/h6H,4-5H2,1-3H3
InchiKey:	ZQAYBCWERYRAMF-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	COCCC(C)C
Mol. weight [g/mol]:	102.17
CAS:	626-91-5

Physical Properties

Property code	Value	Unit	Source
gf	-107.80	kJ/mol	Joback Method
hf	-304.67	kJ/mol	Joback Method
hfus	8.96	kJ/mol	Joback Method
hvap	35.75	kJ/mol	NIST Webbook
ie	9.65	eV	NIST Webbook
log10ws	-1.18		Crippen Method
logp	1.679		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	693.80		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	684.00		NIST Webbook
tb	364.60	K	NIST Webbook
tc	527.06	K	Joback Method
tf	164.61	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.11	J/mol×K	527.06	Joback Method
cpg	181.69	J/mol×K	358.66	Joback Method
cpg	192.17	J/mol×K	386.73	Joback Method
cpg	202.35	J/mol×K	414.79	Joback Method
cpg	212.24	J/mol×K	442.86	Joback Method
cpg	221.82	J/mol×K	470.92	Joback Method
cpg	231.12	J/mol×K	498.99	Joback Method
dvisc	0.0002155	Pa×s	358.66	Joback Method
dvisc	0.0064749	Pa×s	164.61	Joback Method
dvisc	0.0023051	Pa×s	196.95	Joback Method
dvisc	0.0010982	Pa×s	229.29	Joback Method
dvisc	0.0006285	Pa×s	261.63	Joback Method
dvisc	0.0004067	Pa×s	293.98	Joback Method
dvisc	0.0002868	Pa×s	326.32	Joback Method
hvapt	31.29	kJ/mol	364.60	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=C626915&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

ie:	Ionization energy
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