Butane, 1-(1-methylethoxy)-

Other names:	Ether, butyl isopropyl
	Butyl isopropyl ether
Inchi:	InChI=1S/C7H16O/c1-4-5-6-8-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	GPDFVOVLOXMSBT-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCOC(C)C
Mol. weight [g/mol]:	116.20
CAS:	1860-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-99.38	kJ/mol	Joback Method
hf	-325.31	kJ/mol	Joback Method
hfus	11.55	kJ/mol	Joback Method
hvap	38.80	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	725.00		NIST Webbook
tb	382.30	K	NIST Webbook
tc	549.69	K	Joback Method
tf	175.88	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.00	J/mol×K	549.69	Joback Method
cpg	218.33	J/mol×K	381.54	Joback Method
cpg	230.17	J/mol×K	409.57	Joback Method
cpg	241.65	J/mol×K	437.59	Joback Method
cpg	252.77	J/mol×K	465.62	Joback Method
cpg	263.53	J/mol×K	493.64	Joback Method

cpg	273.94	J/mol×K	521.67	Joback Method
dvisc	0.0002162	Pa×s	381.54	Joback Method
dvisc	0.0068890	Pa×s	175.88	Joback Method
dvisc	0.0024170	Pa×s	210.16	Joback Method
dvisc	0.0011375	Pa×s	244.43	Joback Method
dvisc	0.0006444	Pa×s	278.71	Joback Method
dvisc	0.0004135	Pa×s	312.99	Joback Method
dvisc	0.0002896	Pa×s	347.26	Joback Method
hvapt	32.95	kJ/mol	382.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	98.40	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=C1860271&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume