

Butane, 1-(1-methylpropoxy)-

Inchi:	InChI=1S/C8H18O/c1-4-6-7-9-8(3)5-2/h8H,4-7H2,1-3H3
InchiKey:	LPVMPBNUHJKNHA-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCOC(C)CC
Mol. weight [g/mol]:	130.23
CAS:	999-65-5

Physical Properties

Property code	Value	Unit	Source
gf	-90.96	kJ/mol	Joback Method
hf	-345.95	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	35.42	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.602		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
tb	404.42	K	Joback Method
tc	572.04	K	Joback Method
tf	187.15	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.42	J/molxK	404.42	Joback Method
cpg	318.62	J/molxK	544.10	Joback Method
cpg	307.20	J/molxK	516.17	Joback Method
cpg	295.37	J/molxK	488.23	Joback Method
cpg	283.13	J/molxK	460.29	Joback Method
cpg	270.49	J/molxK	432.36	Joback Method
cpg	329.64	J/molxK	572.04	Joback Method
dvisc	0.0002120	Paxs	404.42	Joback Method
dvisc	0.0002854	Paxs	368.21	Joback Method

dvisc	0.0004101	Paxs	332.00	Joback Method
dvisc	0.0006440	Paxs	295.78	Joback Method
dvisc	0.0011469	Paxs	259.57	Joback Method
dvisc	0.0024628	Paxs	223.36	Joback Method
dvisc	0.0071085	Paxs	187.15	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=C999655&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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