

Ether, butyl isopentyl

Other names:	Butane, 1-butoxy-3-methyl- Butyl isopentyl ether butyl 3-methylbutyl ether
Inchi:	InChI=1S/C9H20O/c1-4-5-7-10-8-6-9(2)3/h9H,4-8H2,1-3H3
InchiKey:	NMLLTHLOSVNFMY-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCOCCC(C)C
Mol. weight [g/mol]:	144.25
CAS:	17071-52-2

Physical Properties

Property code	Value	Unit	Source
gf	-82.54	kJ/mol	Joback Method
hf	-366.59	kJ/mol	Joback Method
hfus	16.73	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.849		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
tb	427.30	K	Joback Method
tc	594.17	K	Joback Method
tf	198.42	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.83	J/molxK	427.30	Joback Method
cpg	365.04	J/molxK	566.36	Joback Method
cpg	352.71	J/molxK	538.55	Joback Method
cpg	339.94	J/molxK	510.74	Joback Method
cpg	326.70	J/molxK	482.92	Joback Method
cpg	313.00	J/molxK	455.11	Joback Method

cpg	376.92	J/mol×K	594.17	Joback Method
dvisc	0.0002040	Paxs	427.30	Joback Method
dvisc	0.0002760	Paxs	389.15	Joback Method
dvisc	0.0003988	Paxs	351.01	Joback Method
dvisc	0.0006303	Paxs	312.86	Joback Method
dvisc	0.0011312	Paxs	274.71	Joback Method
dvisc	0.0024518	Paxs	236.57	Joback Method
dvisc	0.0071547	Paxs	198.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17071522&Units=SI

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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