

Butyl 1,1-dimethylpropyl ether

Other names:	butane, 2-butoxy-2-methyl- butyl tert-pentyl ether ether, butyl tert-pentyl
Inchi:	InChI=1S/C9H20O/c1-5-7-8-10-9(3,4)6-2/h5-8H2,1-4H3
InchiKey:	FTGPSKPJRKRPX-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCOC(C)(C)CC
Mol. weight [g/mol]:	144.25
CAS:	3249-47-6

Physical Properties

Property code	Value	Unit	Source
chl	-5971.54 ± 0.90	kJ/mol	NIST Webbook
gf	-77.26	kJ/mol	Joback Method
hf	-382.20 ± 0.93	kJ/mol	NIST Webbook
hfl	-428.34 ± 0.90	kJ/mol	NIST Webbook
hfus	12.84	kJ/mol	Joback Method
hvac	46.10 ± 0.30	kJ/mol	NIST Webbook
hvap	46.14 ± 0.25	kJ/mol	NIST Webbook
hvap	48.30	kJ/mol	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.992		Crippen Method
mccol	143.540	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	424.51	K	Joback Method
tc	598.00	K	Joback Method
tf	215.84	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.63	J/mol×K	598.00	Joback Method
cpg	315.82	J/mol×K	453.43	Joback Method

cpg	330.37	J/molxK	482.34	Joback Method
cpg	344.30	J/molxK	511.26	Joback Method
cpg	357.65	J/molxK	540.17	Joback Method
cpg	370.42	J/molxK	569.09	Joback Method
cpg	300.66	J/molxK	424.51	Joback Method
dvisc	0.0071777	Paxs	215.84	Joback Method
dvisc	0.0027004	Paxs	250.62	Joback Method
dvisc	0.0012893	Paxs	285.40	Joback Method
dvisc	0.0007228	Paxs	320.17	Joback Method
dvisc	0.0004539	Paxs	354.95	Joback Method
dvisc	0.0003097	Paxs	389.73	Joback Method
dvisc	0.0002250	Paxs	424.51	Joback Method
pvap	0.90	kPa	303.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.61	kPa	298.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.74	kPa	301.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.67	kPa	298.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.90	kPa	304.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	1.20	kPa	308.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.55	kPa	296.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.44	kPa	293.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.48	kPa	293.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.36	kPa	290.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.32	kPa	288.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.26	kPa	286.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.25	kPa	285.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.22	kPa	283.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.23	kPa	283.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.18	kPa	281.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.15	kPa	278.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.16	kPa	278.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.13	kPa	276.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.11	kPa	274.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3249476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers:	https://www.doi.org/10.1021/je0255980
Experimental Study of Chemical Thermodynamics of Benzyl Alcohol Reaction Equilibria in Solvents:	https://www.doi.org/10.1021/je034172y
Joback Method:	https://www.doi.org/10.1021/je049823k
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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