Butane, 1,1-diethoxy-

Other names:	Butyraldehyde, diethyl acetal
	Butylaldehyde diethyl acetal
	1,1-Diethoxybutane
	n-Butyraldehyde diethyl acetal
Inchi:	InChI=1S/C8H18O2/c1-4-7-8(9-5-2)10-6-3/h8H,4-7H2,1-3H3
InchiKey:	UVHXZFGCCJLFMX-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CCCC(OCC)OCC
Mol. weight [g/mol]:	146.23
CAS:	3658-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-195.96	kJ/mol	Joback Method
hf	-478.17	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	37.83	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.186		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	880.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	929.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	988.00		NIST Webbook
ripol	1030.00		NIST Webbook
ripol	990.00		NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	416.50 ± 0.50	K	NIST Webbook
tb	416.20	K	NIST Webbook
tc	594.62	K	Joback Method
tf	209.38	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/mol×K	426.84	Joback Method
cpg	295.24	J/mol×K	454.80	Joback Method
cpg	307.70	J/mol×K	482.77	Joback Method
cpg	319.80	J/mol×K	510.73	Joback Method
cpg	331.54	J/mol×K	538.70	Joback Method
cpg	342.91	J/mol×K	566.66	Joback Method
cpg	353.90	J/mol×K	594.62	Joback Method
dvisc	0.0048555	Pa×s	209.38	Joback Method
dvisc	0.0018809	Pa×s	245.62	Joback Method
dvisc	0.0009298	Pa×s	281.87	Joback Method
dvisc	0.0005397	Pa×s	318.11	Joback Method
dvisc	0.0003502	Pa×s	354.35	Joback Method
dvisc	0.0002462	Pa×s	390.60	Joback Method
dvisc	0.0001837	Pa×s	426.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3658955&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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