

Butane, 1,1-dibutoxy-

Other names:	Butyraldehyde, dibutyl acetal Lageracetal 1,1-Dibutoxybutane
Inchi:	InChI=1S/C12H26O2/c1-4-7-10-13-12(9-6-3)14-11-8-5-2/h12H,4-11H2,1-3H3
InchiKey:	WQRBJFZKPWPIJD-UHFFFAOYSA-N
Formula:	C12H26O2
SMILES:	CCCCOC(CCC)OCCCC
Mol. weight [g/mol]:	202.33
CAS:	5921-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-162.28	kJ/mol	Joback Method
hf	-560.73	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.746		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
tb	486.00 ± 5.00	K	NIST Webbook
tc	682.34	K	Joback Method
tf	254.46	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.54	J/mol×K	518.36	Joback Method
cpg	481.08	J/mol×K	545.69	Joback Method
cpg	497.06	J/mol×K	573.02	Joback Method
cpg	512.48	J/mol×K	600.35	Joback Method

cpg	527.34	J/mol×K	627.68	Joback Method
cpg	541.66	J/mol×K	655.01	Joback Method
cpg	555.42	J/mol×K	682.34	Joback Method
dvisc	0.0042647	Pa×s	254.46	Joback Method
dvisc	0.0015728	Pa×s	298.44	Joback Method
dvisc	0.0007494	Pa×s	342.43	Joback Method
dvisc	0.0004228	Pa×s	386.41	Joback Method
dvisc	0.0002681	Pa×s	430.39	Joback Method
dvisc	0.0001850	Pa×s	474.38	Joback Method
dvisc	0.0001359	Pa×s	518.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C5921802&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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