Butane, 1,1-diethoxy-2-methyl-

Other names: Butyraldehyde, 2-methyl-, diethyl acetal
1,1-Diethoxy-2-methylbutane
Inchi: InChI=1S/C9H20O2/c1-5-8(4)9(10-6-2)11-7-3/h8-9H,5-7H2,1-4H3
InchiKey: PAPSQZAQCBGYCJ-UHFFFAOYSA-N
Formula: C9H20O2
SMILES: CCOC(OCC)C(C)CC
Mol. weight [g/mol]: 160.25
CAS: 3658-94-4

Physical Properties

Property code	Value	Unit	Source
gf	-189.98	kJ/mol	Joback Method
hf	-504.09	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	39.67	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.432		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
ripol	1067.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1067.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1067.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1079.00		NIST Webbook
tb	449.28	K	Joback Method
tc	619.70	K	Joback Method
tf	205.65	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.90	J/mol×K	449.28	Joback Method
cpg	339.18	J/mol×K	477.68	Joback Method
cpg	353.03	J/mol×K	506.09	Joback Method
cpg	366.43	J/mol×K	534.49	Joback Method
cpg	379.40	J/mol×K	562.89	Joback Method
cpg	391.92	J/mol×K	591.30	Joback Method
cpg	403.99	J/mol×K	619.70	Joback Method
dvisc	0.0081421	Pa×s	205.65	Joback Method
dvisc	0.0024899	Pa×s	246.25	Joback Method
dvisc	0.0010648	Pa×s	286.86	Joback Method
dvisc	0.0005622	Pa×s	327.47	Joback Method
dvisc	0.0003417	Pa×s	368.07	Joback Method
dvisc	0.0002293	Pa×s	408.67	Joback Method
dvisc	0.0001654	Pa×s	449.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3658944&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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