Butane, 1,1-diethoxy-3-methyl-

Other names:	Isovaleraldehyde, diethyl acetal
	1,1-Diethoxy-3-methylbutane
	3-Methylbutanal, diethyl acetal
	isopentanal diethyl acetal
	1,1-diethoxy-3-methyl butane (isovaleraldehyde diethyl acetal)
Inchi:	InChI=1S/C9H20O2/c1-5-10-9(11-6-2)7-8(3)4/h8-9H,5-7H2,1-4H3
InchiKey:	DDGBOLJFAMEBOE-UHFFFAOYSA-N
Formula:	C9H20O2
SMILES:	CCOC(CC(C)C)OCC
Mol. weight [g/mol]:	160.25
CAS:	3842-03-3

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	952.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1062.00		NIST Webbook

ripol	1065.00		NIST Webbook
ripol	1061.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1074.00		NIST Webbook
ripol	1068.00		NIST Webbook
ripol	1062.00		NIST Webbook
ripol	1062.00		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=C3842033&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