1,3-Dioxolane, 2-butyl-4-methyl-

Other names:	Pentanal propyleneglycol acetal
	1,3-Dioxolane, 4-methyl-2-butyl
	2-Butyl-4-methyl-1,3-dioxolane
	1,3-Dioxolane, 2-butyl-4-methyl, cis
	1,3-Dioxolane, 2-butyl-4-methyl, trans
Inchi:	InChI=1S/C8H16O2/c1-3-4-5-8-9-6-7(2)10-8/h7-8H,3-6H2,1-2H3
InchiKey:	WTZJUXYVLRJTMQ-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCC1OCC(C)O1
Mol. weight [g/mol]:	144.21
CAS:	74094-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-126.92	kJ/mol	Joback Method
hf	-432.31	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	42.37	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.938		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	956.00		NIST Webbook
tb	446.95	K	Joback Method
tc	639.65	K	Joback Method
tf	239.72	K	Joback Method

vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.39	J/mol×K	446.95	Joback Method
cpg	293.17	J/mol×K	479.07	Joback Method
cpg	308.24	J/mol×K	511.18	Joback Method
cpg	322.61	J/mol×K	543.30	Joback Method
cpg	336.31	J/mol×K	575.41	Joback Method
cpg	349.35	J/mol×K	607.53	Joback Method
cpg	361.73	J/mol×K	639.65	Joback Method
dvisc	0.0039167	Pa×s	239.72	Joback Method
dvisc	0.0021065	Pa×s	274.26	Joback Method
dvisc	0.0013015	Pa×s	308.80	Joback Method
dvisc	0.0008859	Pa×s	343.34	Joback Method
dvisc	0.0006470	Pa×s	377.87	Joback Method
dvisc	0.0004980	Pa×s	412.41	Joback Method
dvisc	0.0003992	Pa×s	446.95	Joback Method

Sources

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=C74094603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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