1,3-Dioxolane, 2-hexyl-

Other names:	Ethylene glycol acetal of heptaldehyde
	Heptaldehyde, ethylene glycol acetal
	Heptanal, cyclic ethylene acetal
	Heptanal, cyclic 1,2-ethanediyl acetal
	2-n-Hexyl-1,3-dioxolane
	2-Hexyl-1,3-dioxolane
	n-Heptanal ethyleneglycol acetal
Inchi:	InChI=1S/C9H18O2/c1-2-3-4-5-6-9-10-7-8-11-9/h9H,2-8H2,1H3
InchiKey:	DDSSJDFXTAYRNO-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCC1OCCO1
Mol. weight [g/mol]:	158.24
CAS:	1708-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-110.79	kJ/mol	Joback Method
hf	-432.61	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	44.91	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.330		Crippen Method
mcvol	138.550	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	1460.00		NIST Webbook
tb	469.00 ± 3.00	K	NIST Webbook
tc	665.44	K	Joback Method
tf	255.23	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.33	J/mol×K	474.50	Joback Method
cpg	337.72	J/mol×K	506.32	Joback Method
cpg	353.33	J/mol×K	538.15	Joback Method
cpg	368.18	J/mol×K	569.97	Joback Method
cpg	382.30	J/mol×K	601.80	Joback Method
cpg	395.70	J/mol×K	633.62	Joback Method
cpg	408.41	J/mol×K	665.44	Joback Method
dvisc	0.0058718	Pa×s	255.23	Joback Method
dvisc	0.0027815	Pa×s	291.77	Joback Method
dvisc	0.0015561	Pa×s	328.32	Joback Method
dvisc	0.0009780	Pa×s	364.87	Joback Method
dvisc	0.0006688	Pa×s	401.41	Joback Method
dvisc	0.0004874	Pa×s	437.96	Joback Method
dvisc	0.0003729	Pa×s	474.50	Joback Method
hvapt	55.00	kJ/mol	339.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1708345&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
hvapt: Enthalpy of vaporization at a given temperature

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