1,3-Dioxolane, 2-methyl-2-pentyl-

Other names: 2-Heptanone, cyclic 1,2-ethanediyl acetal
2-Methyl-2-pentyl-1,3-dioxolane
Inchi: InChI=1S/C9H18O2/c1-3-4-5-6-9(2)10-7-8-11-9/h3-8H2,1-2H3
InchiKey: OUQPLRDJDIOBOU-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCCC1(C)OCCO1
Mol. weight [g/mol]: 158.24
CAS: 4352-95-8

Physical Properties

Property code	Value	Unit	Source
gf	-116.28	kJ/mol	Joback Method
hf	-417.37	kJ/mol	Joback Method
hfus	22.66	kJ/mol	Joback Method
hvap	54.00 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.27		Crippen Method
logp	2.330		Crippen Method
mcvol	138.550	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	474.74	K	Joback Method
tc	673.73	K	Joback Method
tf	279.13	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.90	J/mol×K	474.74	Joback Method
cpg	338.44	J/mol×K	507.90	Joback Method
cpg	353.97	J/mol×K	541.07	Joback Method
cpg	368.56	J/mol×K	574.23	Joback Method
cpg	382.31	J/mol×K	607.40	Joback Method
cpg	395.32	J/mol×K	640.56	Joback Method
cpg	407.67	J/mol×K	673.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4352958&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume