1,3-Dioxolane, 2,2-diethyl-

Other names: 3-Pentanone, cyclic 1,2-ethanediyl acetal
2,2-Diethyl-1,3-dioxolane
Inchi: InChI=1S/C7H14O2/c1-3-7(4-2)8-5-6-9-7/h3-6H2,1-2H3
InchiKey: VEMJEYFBPWSPHU-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCC1(CC)OCCO1
Mol. weight [g/mol]: 130.18
CAS: 4362-57-6

Physical Properties

Property code	Value	Unit	Source
gf	-133.12	kJ/mol	Joback Method
hf	-376.09	kJ/mol	Joback Method
hfus	17.48	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.550		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
ripol	1208.00		NIST Webbook
ripol	1208.00		NIST Webbook
tb	428.98	K	Joback Method
tc	632.81	K	Joback Method
tf	256.59	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.68	J/mol×K	428.98	Joback Method
cpg	250.57	J/mol×K	462.95	Joback Method
cpg	264.43	J/mol×K	496.92	Joback Method
cpg	277.36	J/mol×K	530.89	Joback Method
cpg	289.44	J/mol×K	564.86	Joback Method

cpg	300.78	J/mol×K	598.84	Joback Method
cpg	311.46	J/mol×K	632.81	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=C4362576&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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