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

Other names: Propanal, cyclic 1-methyl-1,2-ethanediyl acetal
2-Ethyl-4-methyl-1,3-dioxolane
1,3-Dioxolane, 2-ethyl-4-methyl, cis
Inchi: InChI=1S/C6H12O2/c1-3-6-7-4-5(2)8-6/h5-6H,3-4H2,1-2H3/t5-,6+/m1/s1
InchiKey: CSZCLQLJVFLXLI-RITPCOANSA-N
Formula: C6H12O2
SMILES: CCC1OCC(C)O1
Mol. weight [g/mol]: 116.16
CAS: 4359-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-143.76	kJ/mol	Joback Method
hf	-391.03	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	37.92	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	778.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	778.00		NIST Webbook
tb	401.19	K	Joback Method
tc	597.60	K	Joback Method
tf	217.18	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.22	J/mol×K	401.19	Joback Method

cpg	256.80	J/mol×K	564.86	Joback Method
cpg	245.63	J/mol×K	532.13	Joback Method
cpg	233.89	J/mol×K	499.39	Joback Method
cpg	221.59	J/mol×K	466.66	Joback Method
cpg	208.70	J/mol×K	433.92	Joback Method
cpg	267.43	J/mol×K	597.60	Joback Method
dvisc	0.0004046	Pa×s	401.19	Joback Method
dvisc	0.0004966	Pa×s	370.52	Joback Method
dvisc	0.0006323	Pa×s	339.85	Joback Method
dvisc	0.0008448	Pa×s	309.19	Joback Method
dvisc	0.0012029	Pa×s	278.52	Joback Method
dvisc	0.0018693	Pa×s	247.85	Joback Method
dvisc	0.0032903	Pa×s	217.18	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=C4359460&Units=SI

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