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

Other names:	2-Butanone, cyclic ethylene acetal
	2-Butanone, cyclic 1,2-ethanediyl acetal
	2-Ethyl-2-methyldioxolane
	2-Methyl-2-ethyldioxolane
	2-Ethyl-2-methyl-1,3-dioxolane
	2-Methyl-2-ethyl-1,3-dioxolane
Inchi:	InChI=1S/C6H12O2/c1-3-6(2)7-4-5-8-6/h3-5H2,1-2H3
InchiKey:	UPZFLZYXYGBAPL-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC1(C)OCCO1
Mol. weight [g/mol]:	116.16
CAS:	126-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-141.54	kJ/mol	Joback Method
hf	-355.45	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	44.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.01		Crippen Method
logp	1.159		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	779.00		NIST Webbook
tb	391.20	K	NIST Webbook
tb	391.05	K	NIST Webbook
tb	389.70	K	NIST Webbook
tc	612.10	K	Joback Method
tf	191.19 ± 0.60	K	NIST Webbook
tf	191.15	K	NIST Webbook
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.72	J/mol×K	577.77	Joback Method
cpg	195.53	J/mol×K	406.10	Joback Method
cpg	209.42	J/mol×K	440.43	Joback Method
cpg	222.29	J/mol×K	474.77	Joback Method
cpg	234.24	J/mol×K	509.10	Joback Method
cpg	245.35	J/mol×K	543.43	Joback Method
cpg	265.44	J/mol×K	612.10	Joback Method
hvapt	43.10 ± 0.30	kJ/mol	293.50	NIST Webbook

Sources

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=C126396&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume