1,3-Dioxolane, 2-methyl-2-phenyl-

Other names: Acetophenone ethylene ketal
2-Methyl-2-phenyl-1,3-dioxolane
Inchi: InChI=1S/C10H12O2/c1-10(11-7-8-12-10)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3
InchiKey: GAOQAPRPYXWTFK-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC1(c2ccccc2)OCCO1
Mol. weight [g/mol]: 164.20
CAS: 3674-77-9

Physical Properties

Property code	Value	Unit	Source
chs	-5306.30 ± 2.00	kJ/mol	NIST Webbook
gf	4.55	kJ/mol	Joback Method
hf	-261.90 ± 2.20	kJ/mol	NIST Webbook
hfs	-343.80 ± 2.10	kJ/mol	NIST Webbook
hfus	19.29	kJ/mol	Joback Method
hsub	81.90	kJ/mol	NIST Webbook
hsub	81.88 ± 0.50	kJ/mol	NIST Webbook
hvap	48.26	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.906		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	524.30	K	Joback Method
tc	770.55	K	Joback Method
tf	316.82	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.71	J/mol×K	524.30	Joback Method
cpg	318.41	J/mol×K	565.34	Joback Method
cpg	333.71	J/mol×K	606.38	Joback Method

cpg	347.79	J/mol×K	647.42	Joback Method
cpg	360.86	J/mol×K	688.47	Joback Method
cpg	373.10	J/mol×K	729.51	Joback Method
cpg	384.69	J/mol×K	770.55	Joback Method
hsubt	81.90 ± 0.50	kJ/mol	308.50	NIST Webbook

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=C3674779&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsub: Enthalpy of sublimation at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

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