

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

Physical Properties

Property code	Value	Unit	Source
chs	-5306.30 ± 2.00	kJ/mol	NIST Webbook
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	81.88 ± 0.50	kJ/mol	NIST Webbook
hsub	81.90	kJ/mol	NIST Webbook
ie	8.79	eV	Cheméo Relay (1.0)
logp	1.906		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
tb	477.44	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3674779&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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