

Ethanone, 2,2-dimethoxy-1,2-diphenyl-

Other names:

«alpha», «alpha»-Dimethoxy-«alpha»-phenylacetophenone

2,2-Dimethoxy-2-phenylacetophenone

Benzil dimethyl ketal

DMPA

Photocure 51

2,2-Dimethoxy-1,2-diphenylethanone

Irgacure 651

1,2-Diphenyl-2,2-dimethoxyethanone

2,2-Dimethoxyphenylacetophenone

2-Phenyl-2,2-dimethoxyacetophenone

Benzil dimethyl acetal

Benzil mono(dimethyl acetal)

Benzil mono(dimethyl ketal)

Esacure KB 1

IR 651

IRG 651

Irgacure 621

Irgacure 641

Irgacure E 651

Irgacure I 651

Kayacure BDMK

KB 1

Lucirin BDK

Photomer 51

«alpha», «alpha»-Dimethoxydeoxybenzoin

Irgacure 651 (2,2-Dimethoxy-2-phenylacetophenone)

2,2-dimethoxy-1,2-diphenylethan-1-one

Inchi:

InChI=1S/C16H16O3/c1-18-16(19-2,14-11-7-4-8-12-14)15(17)13-9-5-3-6-10-13/h3-12H,1

InchiKey:

KWVGIIHKZDCUPEU-UHFFFAOYSA-N

Formula:

C16H16O3

SMILES:

COC(OC)(C(=O)c1ccccc1)c1ccccc1

Mol. weight [g/mol]:

256.30

CAS:

24650-42-8

Physical Properties

Property code	Value	Unit	Source
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gf	-27.42		kJ/mol	Joback Method
hf	-286.28		kJ/mol	Joback Method
hfus	21.84		kJ/mol	Joback Method
hvap	66.03		kJ/mol	Joback Method
log10ws	-3.42			Crippen Method
logp	3.015			Crippen Method
mcvol	202.090		ml/mol	McGowan Method
pc	2393.53		kPa	Joback Method
rinpol	1874.00			NIST Webbook
rinpol	1874.00			NIST Webbook
tb	714.32		K	Joback Method
tc	957.06		K	Joback Method
tf	338.50 ± 0.80		K	NIST Webbook
vc	0.747		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.98	J/molxK	714.32	Joback Method
cpg	564.18	J/molxK	754.78	Joback Method
cpg	578.98	J/molxK	795.23	Joback Method
cpg	592.47	J/molxK	835.69	Joback Method
cpg	604.71	J/molxK	876.15	Joback Method
cpg	615.78	J/molxK	916.60	Joback Method
cpg	625.76	J/molxK	957.06	Joback Method
dvisc	0.0010332	Paxs	419.73	Joback Method
dvisc	0.0005381	Paxs	468.83	Joback Method
dvisc	0.0003171	Paxs	517.93	Joback Method
dvisc	0.0002048	Paxs	567.03	Joback Method
dvisc	0.0001418	Paxs	616.12	Joback Method
dvisc	0.0001037	Paxs	665.22	Joback Method
dvisc	0.0000791	Paxs	714.32	Joback Method
hfust	20.86	kJ/mol	338.50	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=C24650428&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
hfust: Enthalpy of fusion 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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