

# Ethanedione, (4-methoxyphenyl)phenyl-

<b>Other names:</b>	Benzil, 4-methoxy- p-Methoxybenzil 4-Methoxybenzil 1-(4-Methoxyphenyl)-2-phenyl-ethan-1,2-dion 1-(4-Methoxyphenyl)-2-phenyl-ethan-1,2-dione 1-(4-Methoxyphenyl)-2-phenyl-1,2-ethanedione Dibenzoyl, 4-methoxy NSC 39465
<b>Inchi:</b>	InChI=1S/C15H12O3/c1-18-13-9-7-12(8-10-13)15(17)14(16)11-5-3-2-4-6-11/h2-10H,1H3
<b>InchiKey:</b>	NTINAJCDYRYMML-UHFFFAOYSA-N
<b>Formula:</b>	C15H12O3
<b>SMILES:</b>	COc1ccc(C(=O)C(=O)c2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	240.25
<b>CAS:</b>	22711-21-3

## Physical Properties

Property code	Value	Unit	Source
gf	-72.23	kJ/mol	Joback Method
hf	-248.72	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.761		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	731.10	K	Joback Method
tc	975.09	K	Joback Method
tf	446.26	K	Joback Method
vc	0.690	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.02	J/molxK	731.10	Joback Method
cpg	536.90	J/molxK	934.42	Joback Method
cpg	527.71	J/molxK	893.76	Joback Method
cpg	517.48	J/molxK	853.09	Joback Method
cpg	506.15	J/molxK	812.43	Joback Method
cpg	493.68	J/molxK	771.76	Joback Method
cpg	545.09	J/molxK	975.09	Joback Method
dvisc	0.0001379	Paxs	731.10	Joback Method
dvisc	0.0001724	Paxs	683.63	Joback Method
dvisc	0.0002229	Paxs	636.15	Joback Method
dvisc	0.0003004	Paxs	588.68	Joback Method
dvisc	0.0004265	Paxs	541.21	Joback Method
dvisc	0.0006479	Paxs	493.73	Joback Method
dvisc	0.0010757	Paxs	446.26	Joback Method

## Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/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=C22711213&Units=SI>

**Crippen Method:**

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

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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