

Ethanedione, (4-methylphenyl)phenyl-

Other names:	p-Methylbenzil 4-Methylbenzil
Inchi:	InChI=1S/C15H12O2/c1-11-7-9-13(10-8-11)15(17)14(16)12-5-3-2-4-6-12/h2-10H,1H3
InchiKey:	QKFICTUTRIMBEX-UHFFFAOYSA-N
Formula:	C15H12O2
SMILES:	<chem>Cc1ccc(C(=O)C(=O)c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	224.25
CAS:	2431-00-7

Physical Properties

Property code	Value	Unit	Source
gf	32.77	kJ/mol	Joback Method
hf	-116.50	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
ie	9.05 ± 0.10	eV	NIST Webbook
log10ws	-4.08		Crippen Method
logp	3.061		Crippen Method
mcvol	177.830	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	708.68	K	Joback Method
tc	956.65	K	Joback Method
tf	424.03	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.00	J/molxK	708.68	Joback Method
cpg	469.10	J/molxK	750.01	Joback Method
cpg	481.98	J/molxK	791.34	Joback Method
cpg	493.73	J/molxK	832.66	Joback Method
cpg	504.40	J/molxK	873.99	Joback Method
cpg	514.09	J/molxK	915.32	Joback Method

cpg	522.85	J/mol×K	956.65	Joback Method
dvisc	0.0014601	Paxs	424.03	Joback Method
dvisc	0.0008600	Paxs	471.47	Joback Method
dvisc	0.0005580	Paxs	518.91	Joback Method
dvisc	0.0003892	Paxs	566.36	Joback Method
dvisc	0.0002871	Paxs	613.80	Joback Method
dvisc	0.0002212	Paxs	661.24	Joback Method
dvisc	0.0001765	Paxs	708.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2431007&Units=SI
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

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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