

Ethandione, bis(p-tolyl)-

Other names:	4,4'-Dimethylbenzil Ethanedione, bis(4-methylphenyl)- di-p-tolyleanedione
Inchi:	InChI=1S/C16H14O2/c1-11-3-7-13(8-4-11)15(17)16(18)14-9-5-12(2)6-10-14/h3-10H,1-2H
InchiKey:	BCWCEHMHCDCJAD-UHFFFAOYSA-N
Formula:	C16H14O2
SMILES:	Cc1ccc(C(=O)C(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	238.28
CAS:	3457-48-5

Physical Properties

Property code	Value	Unit	Source
gf	31.56	kJ/mol	Joback Method
hf	-148.61	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.369		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	736.54	K	Joback Method
tc	980.06	K	Joback Method
tf	447.82	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.86	J/mol×K	736.54	Joback Method
cpg	520.21	J/mol×K	777.13	Joback Method
cpg	533.38	J/mol×K	817.71	Joback Method
cpg	545.44	J/mol×K	858.30	Joback Method
cpg	556.44	J/mol×K	898.89	Joback Method
cpg	566.45	J/mol×K	939.47	Joback Method

cpg	575.54	J/mol×K	980.06	Joback Method
dvisc	0.0011624	Pa×s	447.82	Joback Method
dvisc	0.0007102	Pa×s	495.94	Joback Method
dvisc	0.0004735	Pa×s	544.06	Joback Method
dvisc	0.0003371	Pa×s	592.18	Joback Method
dvisc	0.0002526	Pa×s	640.30	Joback Method
dvisc	0.0001971	Pa×s	688.42	Joback Method
dvisc	0.0001589	Pa×s	736.54	Joback Method

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=C3457485&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
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

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