

1,1'-(p-Phenylene)bis(2-phenylethanedione)

Other names:	1,4-Bis(phenylglyoxaloyl)benzene
Inchi:	InChI=1S/C22H14O4/c23-19(15-7-3-1-4-8-15)21(25)17-11-13-18(14-12-17)22(26)20(24)
InchiKey:	FUEGWHHUYNHBNl-UHFFFAOYSA-N
Formula:	C22H14O4
SMILES:	O=C(C(=O)c1ccc(C(=O)C(=O)c2ccccc2)cc1)c1ccccc1
Mol. weight [g/mol]:	342.34
CAS:	3363-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-53.72	kJ/mol	Joback Method
hf	-249.61	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	99.04	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	3.818		Crippen Method
mcvol	255.840	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	1003.26	K	Joback Method
tc	1267.25	K	Joback Method
tf	629.20	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.55	J/mol×K	1003.26	Joback Method
cpg	790.76	J/mol×K	1223.25	Joback Method
cpg	784.81	J/mol×K	1179.25	Joback Method
cpg	778.15	J/mol×K	1135.25	Joback Method
cpg	770.64	J/mol×K	1091.26	Joback Method
cpg	762.16	J/mol×K	1047.26	Joback Method
cpg	796.13	J/mol×K	1267.25	Joback Method
dvisc	0.0000718	Pa×s	1003.26	Joback Method

dvisc	0.0000900	Pa×s	940.92	Joback Method
dvisc	0.0001164	Pa×s	878.57	Joback Method
dvisc	0.0001567	Pa×s	816.23	Joback Method
dvisc	0.0002214	Pa×s	753.89	Joback Method
dvisc	0.0003332	Pa×s	691.54	Joback Method
dvisc	0.0005435	Pa×s	629.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3363971&Units=SI

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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