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: FUEGWHHUYNHBNI-UHFFFAOYSA-N
Formula: C22H14O4
SMILES: O=C(C(=O)c1ccc(C(=O)C(=O)c2ccccc2)cc1)c1ccccc1
Mol. weight [g/mol]: 342.35

Physical Properties

Property code	Value	Unit	Source
af	0.8228		Cheméo Relay (1.0)
gf	-53.72	kJ/mol	Joback Method
hf	-223.69	kJ/mol	Cheméo Relay (1.0)
hfus	40.87	kJ/mol	Joback Method
hvap	118.35	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-4.97		Cheméo Relay (1.0)
logp	3.818		Crippen Method
mcvol	255.840	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	699.32	K	Cheméo Relay (1.0)
tc	1048.30	K	Cheméo Relay (1.0)
tf	444.99	K	Cheméo Relay (1.0)
tt	425.10 ± 0.10	K	NIST Webbook
vc	0.939	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	790.76	J/mol×K	1223.25	Joback Method
dvisc	0.0005435	Pa×s	629.20	Joback Method
dvisc	0.0003332	Pa×s	691.54	Joback Method
dvisc	0.0002214	Pa×s	753.89	Joback Method
dvisc	0.0001567	Pa×s	816.23	Joback Method
dvisc	0.0001164	Pa×s	878.57	Joback Method
dvisc	0.0000900	Pa×s	940.92	Joback Method
dvisc	0.0000718	Pa×s	1003.26	Joback Method
hfust	32.30	kJ/mol	402.60	NIST Webbook
hfust	32.30	kJ/mol	425.10	NIST Webbook
sfust	76.00	J/mol×K	402.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
sfust: Entropy of fusion at a given temperature

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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