Propane-1,3-dione, 1,3-diphenyl-2-(phenylimino)-

Other names: 1,3-Diphenyl-2-phenylimino-propan-1,3-dione
Inchi: InChI=1S/C21H15NO2/c23-20(16-10-4-1-5-11-16)19(22-18-14-8-3-9-15-18)21(24)17-12-
InchiKey: NMYSMCUGIBQIHP-UHFFFAOYSA-N
Formula: C21H15NO2
SMILES: O=C(C(=Nc1ccccc1)C(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 313.35
CAS: 24416-28-2

Physical Properties

Property code	Value	Unit	Source
hf	80.09	kJ/mol	Joback Method
hvap	86.05	kJ/mol	Joback Method
ie	8.01 ± 0.05	eV	NIST Webbook
log10ws	-5.40		Crippen Method
logp	4.525		Crippen Method
mcvol	244.290	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
tb	944.22	K	Joback Method
tc	1217.67	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24416282&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

hf: Enthalpy of formation 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