1,3-DIPHENYL-2-PHENYLIMINO-PROPAN-1,3-DIO

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]: 313.36

Physical Properties

Property code	Value	Unit	Source
af	0.7158		Cheméo Relay (1.0)
gf	225.39	kJ/mol	Cheméo Relay (1.0, beta)
hf	176.54	kJ/mol	Cheméo Relay (1.0)
hvap	96.74	kJ/mol	Cheméo Relay (1.0)
ie	8.01 ± 0.05	eV	NIST Webbook
log10ws	-4.78		Cheméo Relay (1.0)
logp	4.525		Crippen Method
mcvol	244.290	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
tb	683.72	K	Cheméo Relay (1.0)
tc	1026.45	K	Cheméo Relay (1.0)
tf	378.65	K	Cheméo Relay (1.0)
vc	0.880	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24416282&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
Cheméo Relay (1.0):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
tf:	Normal melting (fusion) point
vc:	Critical Volume