Propane-1,3-dione, 1,3-diphenyl-2-(4-methoxybenzoyl)-

Inchi: InChI=1S/C23H18O4/c1-27-19-14-12-18(13-15-19)23(26)20(21(24)16-8-4-2-5-9-16)22(2

InchiKey: FKAGMSHKOJSCSM-UHFFFAOYSA-N

Formula: C23H18O4

SMILES: COc1ccc(C(=O)C(C(=O)c2ccccc2)C(=O)c2ccccc2)cc1

Mol. weight [g/mol]: 358.39

CAS: 111473-17-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.82	kJ/mol	Joback Method
hf	-295.17	kJ/mol	Joback Method
hfus	39.52	kJ/mol	Joback Method
hvap	96.54	kJ/mol	Joback Method
ie	7.79	eV	NIST Webbook
log10ws	-5.79		Crippen Method
logp	4.260		Crippen Method
mcvol	274.230	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	994.25	K	Joback Method
tc	1251.34	K	Joback Method
tf	597.77	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.86	J/mol×K	994.25	Joback Method
cpg	873.84	J/mol×K	1208.50	Joback Method
cpg	867.72	J/mol×K	1165.65	Joback Method
cpg	860.57	J/mol×K	1122.80	Joback Method
cpg	852.28	J/mol×K	1079.95	Joback Method
cpg	842.75	J/mol×K	1037.10	Joback Method
cpg	879.04	J/mol×K	1251.34	Joback Method
dvisc	0.0000443	Pa×s	994.25	Joback Method

dvisc	0.0000566	Pa×s	928.17	Joback Method
dvisc	0.0000751	Pa×s	862.09	Joback Method
dvisc	0.0001044	Pa×s	796.01	Joback Method
dvisc	0.0001541	Pa×s	729.93	Joback Method
dvisc	0.0002458	Pa×s	663.85	Joback Method
dvisc	0.0004346	Pa×s	597.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111473177&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

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
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