3,4-Dimethyl-5,5-diphenyl-2(5H)-furanone

Inchi: InChI=1S/C18H16O2/c1-13-14(2)18(20-17(13)19,15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3
InchiKey: QXCGXLHXTZBVQU-UHFFFAOYSA-N
Formula: C18H16O2
SMILES: CC1=C(C)C(c2ccccc2)(c2ccccc2)OC1=O
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	158.55	kJ/mol	Joback Method
hf	-100.93	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	69.69	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.823		Crippen Method
mcvol	209.240	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1815.00		NIST Webbook
tb	784.01	K	Joback Method
tc	1055.99	K	Joback Method
tf	500.85	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.81	J/mol×K	784.01	Joback Method
cpg	619.29	J/mol×K	829.34	Joback Method
cpg	636.88	J/mol×K	874.67	Joback Method
cpg	653.81	J/mol×K	920.00	Joback Method
cpg	670.32	J/mol×K	965.33	Joback Method
cpg	686.65	J/mol×K	1010.66	Joback Method
cpg	703.02	J/mol×K	1055.99	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=R587221&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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