2,5-Dihydro-3,5-diphenyl-5-hydroxyfuran-2-one

Inchi: InChI=1S/C16H12O3/c17-15-14(12-7-3-1-4-8-12)11-16(18,19-15)13-9-5-2-6-10-13/h1-11
InchiKey: VYIYKOAKBRGNBW-UHFFFAOYSA-N
Formula: C16H12O3
SMILES: O=C1OC(O)(c2ccccc2)C=C1c1ccccc1
Mol. weight [g/mol]: 252.26
CAS: 40048-04-2

Physical Properties

Property code	Value	Unit	Source
gf	14.52	kJ/mol	Joback Method
hf	-200.41	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	81.26	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.472		Crippen Method
mcvol	186.930	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	825.45	K	Joback Method
tc	1082.47	K	Joback Method
tf	526.61	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.74	J/mol×K	825.45	Joback Method
cpg	559.13	J/mol×K	868.29	Joback Method
cpg	573.06	J/mol×K	911.12	Joback Method
cpg	586.72	J/mol×K	953.96	Joback Method
cpg	600.32	J/mol×K	996.79	Joback Method
cpg	614.06	J/mol×K	1039.63	Joback Method
cpg	628.16	J/mol×K	1082.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40048042&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume