

4,7-Diphenyl-3a,4,7,7a-tetrahydroisobenzofuran-1

Other names:	4,7-Diphenyl-3a,4,7,7a-tetrahydro-2-benzofuran-1,3-dione 3,6-Diphenyl-4-cyclohexene-1,2-dicarboxylic anhydride 4-Cyclohexene-1,2-dicarboxylic anhydride, 3,6-diphenyl-
Inchi:	InChI=1S/C20H16O3/c21-19-17-15(13-7-3-1-4-8-13)11-12-16(18(17)20(22)23-19)14-9-5
InchiKey:	QBTDNXVTAHQRRU-UHFFFAOYSA-N
Formula:	C20H16O3
SMILES:	O=C1OC(=O)C2C(c3ccccc3)C=CC(c3ccccc3)C12
Mol. weight [g/mol]:	304.34
CAS:	20929-46-8

Physical Properties

Property code	Value	Unit	Source
chs	-9759.60 ± 4.20	kJ/mol	NIST Webbook
gf	110.78	kJ/mol	Joback Method
hf	-246.25	kJ/mol	Joback Method
hfus	35.97	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.440		Crippen Method
mcvol	228.130	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	889.06	K	Joback Method
tc	1171.11	K	Joback Method
tf	548.61	K	Joback Method
vc	0.849	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.98	J/mol×K	889.06	Joback Method
cpg	759.68	J/mol×K	936.07	Joback Method
cpg	774.08	J/mol×K	983.08	Joback Method
cpg	786.23	J/mol×K	1030.09	Joback Method
cpg	796.20	J/mol×K	1077.10	Joback Method

cpg	804.05	J/mol×K	1124.10	Joback Method
cpg	809.83	J/mol×K	1171.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20929468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

chs:	Standard solid enthalpy of combustion
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

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