4,7-DIPHENYL-3A,4,7,7A-TETRAHYDROISOBENZ

Other names: 3,6-Diphenyl-4-cyclohexene-1,2-dicarboxylic anhydride
4,7-Diphenyl-3a,4,7,7a-tetrahydro-2-benzofuran-1,3-dione
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

Physical Properties

Property code	Value	Unit	Source
chs	-9759.60 ± 4.20	kJ/mol	NIST Webbook
hfus	35.97	kJ/mol	Joback Method
logp	3.440		Crippen Method
mcvol	228.130	ml/mol	McGowan 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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20929468&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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume