1-Oxa-spiro[4.5]deca-6,9-diene-2,8-dione, 7,9-di-tert-butyl-

Other names: 1-Oxa-spiro[4.5]deca-6,9-diene-2,8-dione, 7,9-di-tert-butyl-
7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione

Inchi: InChI=1S/C17H24O3/c1-15(2,3)11-9-17(8-7-13(18)20-17)10-12(14(11)19)16(4,5)6/h9-10

InchiKey: ZTMZUYHXZPUDRF-UHFFFAOYSA-N

Formula: C17H24O3

SMILES: CC(C)(C)C1=CC2(C=C(C(C)(C)C)C1=O)CCC(=O)O2

Mol. weight [g/mol]: 276.38

Physical Properties

Property code	Value	Unit	Source
hfus	14.12	kJ/mol	Joback Method
logp	3.590		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
rinpol	1929.00		NIST Webbook
rinpol	1916.80		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1916.80		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.43	J/mol×K	788.24	Joback Method
cpg	741.13	J/mol×K	830.88	Joback Method
cpg	760.84	J/mol×K	873.52	Joback Method
cpg	779.80	J/mol×K	916.16	Joback Method
cpg	798.21	J/mol×K	958.81	Joback Method
cpg	816.28	J/mol×K	1001.45	Joback Method
cpg	834.24	J/mol×K	1044.09	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=C82304663&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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices