

7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione

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]:	276.37
CAS:	82304-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-117.38	kJ/mol	Joback Method
hf	-569.95	kJ/mol	Joback Method
hfus	14.12	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.590		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1916.80		NIST Webbook
rinpol	1916.80		NIST Webbook
tb	788.24	K	Joback Method
tc	1044.09	K	Joback Method
tf	525.70	K	Joback Method
vc	0.854	m3/kmol	Joback Method

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

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=C82304663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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