Benzo[b]-7-oxa-bicyclo[2,2,2]oct-2-en-5(exo),6(exo)-dicarboxylic acid, 4-methyl-1-phenyl, dimethyl ester

Inchi: InChI=1S/C22H22O5/c1-21-13-17-22(14-9-5-4-6-10-14,16-12-8-7-11-15(16)21)18(20(24)

InchiKey: YNXYGYKASMZFRX-KPAFHJTJSA-N

Formula: C22H22O5

SMILES: COC(=O)C1C(C(=O)OC)C2(c3ccccc3)OCC1(C)c1ccccc12

Mol. weight [g/mol]: 366.41

Physical Properties

Property code	Value	Unit	Source
gf	-109.31	kJ/mol	Joback Method
hf	-522.02	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.810		Crippen Method
mcvol	272.350	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
ripol	2938.00		NIST Webbook
ripol	2938.00		NIST Webbook
tb	945.25	K	Joback Method
tc	1195.33	K	Joback Method
tf	649.15	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.41	J/mol×K	945.25	Joback Method
cpg	928.73	J/mol×K	986.93	Joback Method
cpg	953.14	J/mol×K	1028.61	Joback Method
cpg	979.00	J/mol×K	1070.29	Joback Method
cpg	1006.71	J/mol×K	1111.97	Joback Method
cpg	1036.65	J/mol×K	1153.65	Joback Method
cpg	1069.20	J/mol×K	1195.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487953&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume