Trans-1,3-cyclobutanediol-2,2,4,4-tetramethyl-, dibenzoate

InChI: InChI=1S/C22H24O4/c1-21(2)19(25-17(23)15-11-7-5-8-12-15)22(3,4)20(21)26-18(24)16-
InchiKey: FODBNEVOMVOTBG-UHFFFAOYSA-N
Formula: C22H24O4
SMILES: CC1(C)C(OC(=O)c2ccccc2)C(C)(C)C1OC(=O)c1ccccc1
Mol. weight [g/mol]: 352.42
CAS: 95164-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-94.12	kJ/mol	Joback Method
hf	-477.85	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.504		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
tb	906.18	K	Joback Method
tc	1151.67	K	Joback Method
tf	584.36	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.66	J/mol×K	906.18	Joback Method
cpg	919.02	J/mol×K	947.09	Joback Method
cpg	941.71	J/mol×K	988.01	Joback Method
cpg	965.03	J/mol×K	1028.92	Joback Method
cpg	989.29	J/mol×K	1069.84	Joback Method
cpg	1014.80	J/mol×K	1110.75	Joback Method
cpg	1041.88	J/mol×K	1151.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95164719&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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