Benzoic acid, 4,4'-sulfonylbis-, dimethyl ester

Other names:	Benzoic acid, 4,4'-sulfonyldi-, dimethyl ester
	Dimethyl 4,4'-sulfonyldibenzoate
	4,4'-Sulfonylbis(methyl benzoate)
	Benzoic acid, sulfonyl di-p,p'-dimethyl ester
	dimethyl 4,4'-sulphonyldibenzoate
Inchi:	InChI=1S/C16H14O6S/c1-21-15(17)11-3-7-13(8-4-11)23(19,20)14-9-5-12(6-10-14)16(18
InchiKey:	YQYRQRUZQNRJIW-UHFFFAOYSA-N
Formula:	C16H14O6S
SMILES:	COC(=O)c1ccc(S(=O)(=O)c2ccc(C(=O)OC)cc2)cc1
Mol. weight [g/mol]:	334.34
CAS:	3965-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-646.98	kJ/mol	Joback Method
hf	-866.40	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.093		Crippen Method
mcvol	231.750	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	829.16	K	Joback Method
tc	1057.74	K	Joback Method
tf	530.84	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.40	J/mol×K	829.16	Joback Method
cpg	655.30	J/mol×K	867.26	Joback Method
cpg	665.82	J/mol×K	905.35	Joback Method
cpg	674.94	J/mol×K	943.45	Joback Method

cpg	682.67	J/mol×K	981.54	Joback Method
cpg	689.01	J/mol×K	1019.64	Joback Method
cpg	693.95	J/mol×K	1057.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3965535&Units=SI

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