4,4'-Sulfonyldiphthalic dianhydride

Other names:	Bis-(3-phthalyl anhydride) sulfone
	4,4'-Diphthalic anhydride sulfone
	3,3',4,4'-Diphenyl sulfone tetracarboxylic anhydride
	1,3-Isobenzofurandione, 5,5'-sulfonylbis-
Inchi:	InChI=1S/C16H6O8S/c17-13-9-3-1-7(5-11(9)15(19)23-13)25(21,22)8-2-4-10-12(6-8)16(2
InchiKey:	ZHBXLZQQVCDGPA-UHFFFAOYSA-N
Formula:	C16H6O8S
SMILES:	O=C1OC(=O)c2cc(S(=O)(=O)c3ccc4c(c3)C(=O)OC4=O)ccc21
Mol. weight [g/mol]:	358.28
CAS:	2540-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-724.08	kJ/mol	Joback Method
hf	-1028.26	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	103.50	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	1.141		Crippen Method
mcvol	213.170	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
ss	360.70	J/mol×K	NIST Webbook
tb	1034.54	K	Joback Method
tc	1315.20	K	Joback Method
tf	781.94	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.05	J/mol×K	1034.54	Joback Method
cpg	654.99	J/mol×K	1081.32	Joback Method
cpg	656.29	J/mol×K	1128.09	Joback Method
cpg	654.89	J/mol×K	1174.87	Joback Method

cpg	650.68	J/mol×K	1221.65	Joback Method
cpg	643.57	J/mol×K	1268.43	Joback Method
cpg	633.48	J/mol×K	1315.20	Joback Method
cps	360.00	J/mol×K	300.00	NIST Webbook

Sources

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=C2540990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume