bisphenol S

Other names: 4,4'-dihydroxydiphenyl sulfone
4,4'-sulfonyldiphenol
p,p'-dihydroxydiphenyl sulfone
Inchi: InChI=1S/C12H10O4S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8,13-14H
InchiKey: VPWNQTHUCYMVMZ-UHFFFAOYSA-N
Formula: C12H10O4S
SMILES: O=S(=O)(c1ccc(O)cc1)c1ccc(O)cc1
Mol. weight [g/mol]: 250.28

Physical Properties

Property code	Value	Unit	Source
hf	-437.38	kJ/mol	Cheméo Relay (1.0)
hfus	37.86	kJ/mol	Joback Method
hvap	144.59	kJ/mol	Cheméo Relay (1.0)
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	1.931		Crippen Method
mcvol	172.250	ml/mol	McGowan Method
tb	673.27	K	Cheméo Relay (1.0)
tf	480.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.66	J/mol×K	736.34	Joback Method
cpg	466.01	J/mol×K	778.73	Joback Method
cpg	476.51	J/mol×K	821.12	Joback Method
cpg	486.34	J/mol×K	863.52	Joback Method
cpg	495.66	J/mol×K	905.91	Joback Method
cpg	504.65	J/mol×K	948.30	Joback Method
cpg	513.50	J/mol×K	990.69	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility Measurement and Modeling of 4,4'-Dihydroxydiphenyl Sulfone in Nine Organic Solvents from T = (278.15 to 313.15) K and Thermodynamic Property of Dissolution:	https://www.doi.org/10.1021/acs.jced.5b00714
Solubility Determination and Modeling for 4,4'-Dihydroxydiphenyl Sulfone in (Acetone, Ethyl Acetate, or Acetonitrile) + Methanol and Acetone + Ethanol from (278.15 to 313.15) K:	https://www.doi.org/10.1021/acs.jced.6b00421
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point