1,2-Bis(phenylsulfonyl)ethane

Other names: Benzene, 1,1'-[1,2-ethanediylbis(sulfonyl)]bis-
1,2-Bis(phenylsulphonyl)ethane
1,1'-[ethane-1,2-diylbis(sulphonyl)]bisbenzene
Inchi: InChI=1S/C14H14O4S2/c15-19(16,13-7-3-1-4-8-13)11-12-20(17,18)14-9-5-2-6-10-14/h1-
InchiKey: ULELOBVZIKJPAC-UHFFFAOYSA-N
Formula: C14H14O4S2
SMILES: O=S(=O)(CCS(=O)(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 310.39
CAS: 599-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-645.26	kJ/mol	Joback Method
hf	-765.93	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.934		Crippen Method
mcvol	216.780	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	668.64	K	Joback Method
tc	888.27	K	Joback Method
tf	377.50	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.89	J/mol×K	668.64	Joback Method
cpg	560.90	J/mol×K	705.24	Joback Method
cpg	575.57	J/mol×K	741.85	Joback Method
cpg	588.92	J/mol×K	778.45	Joback Method
cpg	600.98	J/mol×K	815.06	Joback Method
cpg	611.78	J/mol×K	851.66	Joback Method

cpg	621.32	J/mol×K	888.27	Joback Method

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=C599940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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