(E)-(2-Phenylethenyl)-sulphonylbenzene

Inchi: InChI=1S/C14H12O2S/c15-17(16,14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-12H/b12-1
InchiKey: DNMCCXFLTURVLK-VAWYXSNFSA-N
Formula: C14H12O2S
SMILES: O=S(=O)(C=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 244.31
CAS: 16212-06-9

Physical Properties

Property code	Value	Unit	Source
chs	-7686.40 ± 2.80	kJ/mol	NIST Webbook
gf	-96.50	kJ/mol	Joback Method
hf	-35.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-139.70 ± 2.90	kJ/mol	NIST Webbook
hfus	31.68	kJ/mol	Joback Method
hsub	105.00 ± 2.00	kJ/mol	NIST Webbook
hvap	69.90	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.131		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	625.02	K	Joback Method
tc	863.99	K	Joback Method
tf	333.86	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.76	J/mol×K	625.02	Joback Method
cpg	453.16	J/mol×K	664.85	Joback Method
cpg	468.18	J/mol×K	704.68	Joback Method
cpg	481.87	J/mol×K	744.50	Joback Method
cpg	494.32	J/mol×K	784.33	Joback Method
cpg	505.60	J/mol×K	824.16	Joback Method

cpg	515.77	J/mol×K	863.99	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=C16212069&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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