Diphenyl sulfoxide

Other names:	Benzene, 1,1'-sulfinylbis-
	Phenyl sulfoxide
	Phenylsulfinylbenzene
	Sulfoxide, diphenyl
	Diphenyl sulphoxide
Inchi:	InChI=1S/C12H10OS/c13-14(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	JJHHIJFTHRNPIK-UHFFFAOYSA-N
Formula:	C12H10OS
SMILES:	O=S(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	202.27
CAS:	945-51-7

Physical Properties

Property code	Value	Unit	Source
chs	-6763.40 ± 0.40	kJ/mol	NIST Webbook
gf	57.27	kJ/mol	Joback Method
hf	107.00 ± 3.00	kJ/mol	NIST Webbook
hfs	10.00 ± 1.00	kJ/mol	NIST Webbook
hfus	22.67	kJ/mol	Joback Method
hsub	97.00 ± 3.00	kJ/mol	NIST Webbook
hvap	59.58	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.58	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.02 ± 0.05	eV	NIST Webbook
log10ws	-2.64		Crippen Method
logp	2.853		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	585.60	K	Joback Method
tc	839.81	K	Joback Method
tf	343.00 ± 3.00	K	NIST Webbook
tf	344.00 ± 3.00	K	NIST Webbook
tf	342.55 ± 0.60	K	NIST Webbook
tf	342.15 ± 1.50	K	NIST Webbook
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.57	J/mol×K	797.44	Joback Method
cpg	344.78	J/mol×K	585.60	Joback Method
cpg	360.74	J/mol×K	627.97	Joback Method
cpg	375.34	J/mol×K	670.34	Joback Method
cpg	388.63	J/mol×K	712.71	Joback Method
cpg	400.69	J/mol×K	755.08	Joback Method
cpg	421.33	J/mol×K	839.81	Joback Method
cps	239.70	J/mol×K	298.50	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=C945517&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
ie: Ionization energy
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