Diphenyl sulfone

Other names:	(Phenylsulfonyl)benzene
	Benzene, 1,1'-sulfonylbis-
	DPS
	Difenylsulfon
	Diphenyl sulphone
	NSC 627706
	NSC 6780
	Phenyl sulfone
	Phenyl sulphone
	Sulfobenzide
	Sulfone, diphenyl
Inchi:	InChI=1S/C12H10O2S/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	KZTYYGOKRVBIMI-UHFFFAOYSA-N
Formula:	C12H10O2S
SMILES:	O=S(=O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	218.27
CAS:	127-63-9

Physical Properties

Property code	Value	Unit	Source
chs	-6528.50 ± 1.50	kJ/mol	NIST Webbook
gf	-193.56	kJ/mol	Joback Method
hf	-118.70 ± 3.30	kJ/mol	NIST Webbook
hfs	-225.00 ± 1.60	kJ/mol	NIST Webbook
hfus	26.30	kJ/mol	Joback Method
hsub	106.00 ± 2.00	kJ/mol	NIST Webbook
hvap	65.49	kJ/mol	Joback Method
ie	9.46	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.16 ± 0.03	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
log10ws	-3.64		Aqueous Solubility Prediction Method
logp	2.519		Crippen Method
mcvol	160.510	ml/mol	McGowan Method

pc	4146.27	kPa	Joback Method
tb	575.10	K	Joback Method
tc	813.46	K	Joback Method
tf	399.00 ± 3.00	K	NIST Webbook
tf	397.00 ± 3.00	K	NIST Webbook
tf	396.00 ± 4.00	K	NIST Webbook
tf	399.00 ± 3.00	K	NIST Webbook
tf	401.00 ± 2.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	398.00 ± 2.00	K	NIST Webbook
tf	400.35 ± 0.60	K	NIST Webbook
tf	397.00 ± 3.00	K	NIST Webbook
tf	400.00 ± 3.00	K	NIST Webbook
tf	397.00 ± 3.00	K	NIST Webbook
tf	433.50 ± 1.50	K	NIST Webbook
tf	397.00 ± 2.00	K	NIST Webbook
tf	398.20	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	401.40	K	Aqueous Solubility Prediction Method
tf	399.00 ± 3.00	K	NIST Webbook
tf	401.40 ± 1.00	K	NIST Webbook
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.96	J/mol×K	773.73	Joback Method
cpg	359.51	J/mol×K	575.10	Joback Method
cpg	375.47	J/mol×K	614.83	Joback Method
cpg	390.15	J/mol×K	654.55	Joback Method
cpg	403.60	J/mol×K	694.28	Joback Method
cpg	415.85	J/mol×K	734.01	Joback Method
cpg	436.97	J/mol×K	813.46	Joback Method
cps	244.30	J/mol×K	298.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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