

Benzene, 1,1'-sulfonylbis[4-chloro-

Other names:	Sulfone, bis(p-chlorophenyl) p,p'-Dichlorodiphenyl sulfone Bis(p-chlorophenyl) sulfone Bis(4-chlorophenyl) sulfone 4-Chloro-1-(4-chlorophenylsulfonyl)benzene 4-Chlorophenyl sulfone 4,4'-Dichlorodiphenyl sulfone p-Chlorophenyl sulfone 4,4'-Dichlorodiphenyl sulphone Bis(4-chlorophenyl)sulphone 1,1'-Sulfonylbis(4-chlorobenzene) Di-p-chlorophenyl sulfone NSC 23899 1-Chloro-4-[(4-chlorophenyl)sulfonyl]benzene 85228-26-8
Inchi:	InChI=1S/C12H8Cl2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H
InchiKey:	GPAPPPVRLPGFEQ-UHFFFAOYSA-N
Formula:	C12H8Cl2O2S
SMILES:	O=S(=O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	287.16
CAS:	80-07-9

Physical Properties

Property code	Value	Unit	Source
gf	-236.68	kJ/mol	Joback Method
hf	-325.72	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.826		Crippen Method
mcvol	184.990	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2270.00		NIST Webbook
ss	314.20	J/mol×K	NIST Webbook

tb	659.92	K	Joback Method
tc	906.63	K	Joback Method
tf	421.90 ± 3.00	K	NIST Webbook
tt	422.00 ± 2.00	K	NIST Webbook
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.18	J/mol×K	906.63	Joback Method
cpg	460.91	J/mol×K	865.51	Joback Method
cpg	408.35	J/mol×K	659.92	Joback Method
cpg	421.14	J/mol×K	701.04	Joback Method
cpg	432.76	J/mol×K	742.16	Joback Method
cpg	443.24	J/mol×K	783.27	Joback Method
cpg	452.61	J/mol×K	824.39	Joback Method
cps	269.30	J/mol×K	298.15	NIST Webbook
hfust	24.40	kJ/mol	422.00	NIST Webbook
hfust	24.40	kJ/mol	422.00	NIST Webbook
hfust	24.40	kJ/mol	422.00	NIST Webbook
hvapt	59.70	kJ/mol	518.00	NIST Webbook
sfust	57.80	J/mol×K	422.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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