

Benzene, 1-fluoro-4-(phenylsulfonyl)-

Other names: 1-fluoro-4-(phenylsulphonyl)benzene;
4-Fluorodiphenylsulfone; 4-Fluorophenyl phenyl sulfone; Sulfone,
p-fluorophenyl phenyl; p-Fluorophenyl phenyl sulfone.

InChI: InChI=1S/C12H9FO2S/c13-10-6-8-12(9-7-10)16(14,15)11-4-2-1-3-5-11/h1-9H

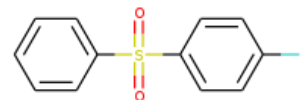
InChI Key: MONGUDQJUIVFPI-UHFFFAOYSA-N

Formula: C12H9FO2S

SMILES: O=S(=O)(c1ccccc1)c1ccc(F)cc1

Molecular Weight: 236.26

CAS: 312-31-2



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-398.00	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-478.88	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	28.99	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	65.34	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.66		Crippen Method
P_c	3843.54	kPa	Joback Method
T_{boil}	579.35	K	Joback Method
T_c	806.80	K	Joback Method
T_{fus}	329.51	K	Joback Method
V_c	0.64	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	367.28	J/mol×K	579.35	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H9FO2S/c13-10-6-8-12\(9-7-10\)16\(14,15\)11-4-2-1-3-5-11/h1-9H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H9FO2S/c13-10-6-8-12(9-7-10)16(14,15)11-4-2-1-3-5-11/h1-9H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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