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

Other names:	Sulfone, p-fluorophenyl phenyl
	p-Fluorophenyl phenyl sulfone
	4-Fluorodiphenylsulfone
	4-Fluorophenyl phenyl sulfone
	1-fluoro-4-(phenylsulphonyl)benzene
Inchi:	InChI=1S/C12H9FO2S/c13-10-6-8-12(9-7-10)16(14,15)11-4-2-1-3-5-11/h1-9H
InchiKey:	MONGUDQJUIVFPI-UHFFFAOYSA-N
Formula:	C12H9FO2S
SMILES:	O=S(=O)(c1ccccc1)c1ccc(F)cc1
Mol. weight [g/mol]:	236.26
CAS:	312-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-398.00	kJ/mol	Joback Method
hf	-478.88	kJ/mol	Joback Method
hfus	28.99	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.658		Crippen Method
mcvol	162.280	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	579.35	K	Joback Method
tc	806.80	K	Joback Method
tf	329.51	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.28	J/mol×K	579.35	Joback Method
cpg	382.11	J/mol×K	617.26	Joback Method
cpg	395.82	J/mol×K	655.17	Joback Method
cpg	408.44	J/mol×K	693.07	Joback Method

cpg	420.00	J/mol×K	730.98	Joback Method
cpg	430.55	J/mol×K	768.89	Joback Method
cpg	440.10	J/mol×K	806.80	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=C312312&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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