

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

Other names:	1-fluoro-4-(methylsulfonyl)benzene
	1-fluoro-4-(methylsulphonyl)benzene
	1-fluoro-4-methanesulfonylbenzene
	1-fluoro-4-methylsulfonylbenzene
	4-(methylsulfonyl)fluorobenzene
	4-fluoro-1-(methylsulfonyl)benzene
	4-fluorophenyl methyl sulfone
	4-methylsulfonyl-1-fluorobenzene
	Sulfone, p-fluorophenyl methyl
	methyl 4-fluorophenyl sulfone
Inchi:	InChI=1S/C7H7FO2S/c1-11(9,10)7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	DPJHZJGAGIWXTD-UHFFFAOYSA-N
Formula:	C7H7FO2S
SMILES:	CS(=O)(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	174.19
CAS:	455-15-2

Physical Properties

Property code	Value	Unit	Source
gf	-552.51	kJ/mol	Joback Method
hf	-612.21	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.229		Crippen Method
mcvol	115.590	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	438.27	K	Joback Method
tc	634.72	K	Joback Method
tf	246.74	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.64	J/mol×K	438.27	Joback Method
cpg	228.71	J/mol×K	471.01	Joback Method
cpg	239.23	J/mol×K	503.75	Joback Method
cpg	249.22	J/mol×K	536.49	Joback Method
cpg	258.68	J/mol×K	569.23	Joback Method
cpg	267.62	J/mol×K	601.98	Joback Method
cpg	276.02	J/mol×K	634.72	Joback Method

Sources

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=C455152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 1-Fluoro-4-(methylsulfonyl)benzene in Five Pure Organic Solvents at Temperatures from (288.40 to 331.50) K:	https://www.doi.org/10.1021/je400965y

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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