5-Fluoro-2-methylbenzenesulphonyl chloride

Inchi: InChI=1S/C7H6ClFO2S/c1-5-2-3-6(9)4-7(5)12(8,10)11/h2-4H,1H3
InchiKey: NPEWBMJAUUSBLE-UHFFFAOYSA-N
Formula: C7H6ClFO2S
SMILES: Cc1ccc(F)cc1S(=O)(=O)Cl
Mol. weight [g/mol]: 208.64
CAS: 445-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-574.07	kJ/mol	Joback Method
hf	-639.42	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	56.98	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.062		Crippen Method
mcvol	127.830	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	480.68	K	Joback Method
tc	684.71	K	Joback Method
tf	289.18	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.74	J/mol×K	480.68	Joback Method
cpg	252.88	J/mol×K	514.68	Joback Method
cpg	262.50	J/mol×K	548.69	Joback Method
cpg	271.59	J/mol×K	582.69	Joback Method
cpg	280.16	J/mol×K	616.70	Joback Method
cpg	288.21	J/mol×K	650.70	Joback Method
cpg	295.73	J/mol×K	684.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C445056&Units=SI
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

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