2-Fluorothiophenol

Inchi: InChI=1S/C6H5FS/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey: WJTZZPVVTSDNJJ-UHFFFAOYSA-N
Formula: C6H5FS
SMILES: Fc1ccccc1S
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
hf	-116.78	kJ/mol	Cheméo Relay (1.0)
hfus	12.07	kJ/mol	Joback Method
hvap	49.46	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	2.114		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
tb	428.06	K	Cheméo Relay (1.0)
tc	667.14	K	Cheméo Relay (1.0)
tf	241.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.19	J/mol×K	430.47	Joback Method
cpg	161.54	J/mol×K	468.89	Joback Method
cpg	170.29	J/mol×K	507.31	Joback Method
cpg	178.46	J/mol×K	545.74	Joback Method
cpg	186.08	J/mol×K	584.16	Joback Method
cpg	193.16	J/mol×K	622.58	Joback Method
cpg	199.74	J/mol×K	661.00	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2557780&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point