3-Chloro-4-fluorothiobenzamide

Inchi: InChI=1S/C7H5ClFNS/c8-5-3-4(7(10)11)1-2-6(5)9/h1-3H,(H2,10,11)
InchiKey: RSGPCKCTKDCMRR-UHFFFAOYSA-N
Formula: C7H5ClFNS
SMILES: NC(=S)c1ccc(F)c(Cl)c1
Mol. weight [g/mol]: 189.64
CAS: 130560-97-3

Physical Properties

Property code	Value	Unit	Source
gf	77.98	kJ/mol	Joback Method
hf	-5.78	kJ/mol	Joback Method
hfus	24.23	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.113		Crippen Method
mcvol	121.770	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	575.47	K	Joback Method
tc	825.12	K	Joback Method
tf	368.15	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.77	J/mol×K	575.47	Joback Method
cpg	250.09	J/mol×K	617.08	Joback Method
cpg	257.68	J/mol×K	658.69	Joback Method
cpg	264.60	J/mol×K	700.30	Joback Method
cpg	270.95	J/mol×K	741.90	Joback Method
cpg	276.79	J/mol×K	783.51	Joback Method
cpg	282.20	J/mol×K	825.12	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=C130560973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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