2-Chloro-6-fluorobenzyl mercaptan

Inchi: InChI=1S/C7H6ClFS/c8-6-2-1-3-7(9)5(6)4-10/h1-3,10H,4H2
InchiKey: TXFPTJWQPHMUEF-UHFFFAOYSA-N
Formula: C7H6ClFS
SMILES: Fc1cccc(Cl)c1CS
Mol. weight [g/mol]: 176.64
CAS: 170924-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-76.14	kJ/mol	Joback Method
hf	-147.59	kJ/mol	Joback Method
hfus	18.47	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.909		Crippen Method
mcvol	116.090	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	495.76	K	Joback Method
tc	730.27	K	Joback Method
tf	287.08	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.58	J/mol×K	495.76	Joback Method
cpg	222.27	J/mol×K	534.85	Joback Method
cpg	231.35	J/mol×K	573.93	Joback Method
cpg	239.82	J/mol×K	613.02	Joback Method
cpg	247.72	J/mol×K	652.10	Joback Method
cpg	255.07	J/mol×K	691.19	Joback Method
cpg	261.89	J/mol×K	730.27	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=C170924524&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