4-Fluorobenzyl mercaptan

Other names: Benzenemethanethiol, 4-fluoro-
p-fluorotoluene-«alpha»-thiol
Inchi: InChI=1S/C7H7FS/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2
InchiKey: RKTRHMNWVZRZJQ-UHFFFAOYSA-N
Formula: C7H7FS
SMILES: Fc1ccc(CS)cc1
Mol. weight [g/mol]: 142.19
CAS: 15894-04-9

Physical Properties

Property code	Value	Unit	Source
gf	-54.58	kJ/mol	Joback Method
hf	-120.38	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.256		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	453.35	K	Joback Method
tc	680.44	K	Joback Method
tf	244.64	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.92	J/mol×K	453.35	Joback Method
cpg	200.73	J/mol×K	491.20	Joback Method
cpg	210.87	J/mol×K	529.05	Joback Method
cpg	220.35	J/mol×K	566.89	Joback Method
cpg	229.22	J/mol×K	604.74	Joback Method
cpg	237.48	J/mol×K	642.59	Joback Method
cpg	245.18	J/mol×K	680.44	Joback Method

Sources

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=C15894049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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