2-Fluorophenoxathiin

Inchi: InChI=1S/C12H7FOS/c13-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)14-10/h1-7H
InchiKey: UKZYOLQBLTVVRO-UHFFFAOYSA-N
Formula: C12H7FOS
SMILES: Fc1ccc2c(c1)Sc1ccccc1O2
Mol. weight [g/mol]: 218.25
CAS: 1800-40-4

Physical Properties

Property code	Value	Unit	Source
gf	85.58	kJ/mol	Joback Method
hf	-35.91	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-4.10		Crippen Method
logp	4.083		Crippen Method
mcvol	145.550	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	623.45	K	Joback Method
tc	881.35	K	Joback Method
tf	451.71	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.44	J/mol×K	623.45	Joback Method
cpg	349.51	J/mol×K	666.43	Joback Method
cpg	360.51	J/mol×K	709.42	Joback Method
cpg	370.56	J/mol×K	752.40	Joback Method
cpg	379.79	J/mol×K	795.39	Joback Method
cpg	388.32	J/mol×K	838.37	Joback Method
cpg	396.30	J/mol×K	881.35	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=C1800404&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
ie:	Ionization energy
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