2,2'-Thiobis[4-fluorophenol]

Inchi: InChI=1S/C12H8F2O2S/c13-7-1-3-9(15)11(5-7)17-12-6-8(14)2-4-10(12)16/h1-6,15-16H
InchiKey: QAEAOHFXMHQPCG-UHFFFAOYSA-N
Formula: C12H8F2O2S
SMILES: Oc1ccc(F)cc1Sc1cc(F)ccc1O
Mol. weight [g/mol]: 254.25
CAS: 401-14-9

Physical Properties

Property code	Value	Unit	Source
gf	-410.02	kJ/mol	Joback Method
hf	-545.86	kJ/mol	Joback Method
hfus	36.00	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.527		Crippen Method
mcvol	164.050	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	765.84	K	Joback Method
tc	1026.09	K	Joback Method
tf	561.90	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.87	J/mol×K	765.84	Joback Method
cpg	439.96	J/mol×K	809.21	Joback Method
cpg	449.54	J/mol×K	852.59	Joback Method
cpg	458.81	J/mol×K	895.96	Joback Method
cpg	467.94	J/mol×K	939.34	Joback Method
cpg	477.14	J/mol×K	982.71	Joback Method
cpg	486.58	J/mol×K	1026.09	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=C401149&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