2,2'-Spirobi[1,3-benzodithiole]

Inchi: InChI=1S/C13H8S4/c1-2-6-10-9(5-1)14-13(15-10)16-11-7-3-4-8-12(11)17-13/h1-8H
InchiKey: ABPUPZOZRITZGO-UHFFFAOYSA-N
Formula: C13H8S4
SMILES: c1ccc2c(c1)SC1(S2)Sc2ccccc2S1
Mol. weight [g/mol]: 292.46
CAS: 837-01-4

Physical Properties

Property code	Value	Unit	Source
gf	559.40	kJ/mol	Joback Method
hf	506.85	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
log10ws	-6.23		Crippen Method
logp	5.394		Crippen Method
mcvol	190.190	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	765.60	K	Joback Method
tc	1100.36	K	Joback Method
tf	715.49	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.93	J/mol×K	765.60	Joback Method
cpg	461.45	J/mol×K	821.39	Joback Method
cpg	475.28	J/mol×K	877.19	Joback Method
cpg	490.18	J/mol×K	932.98	Joback Method
cpg	506.91	J/mol×K	988.77	Joback Method
cpg	526.25	J/mol×K	1044.57	Joback Method
cpg	548.95	J/mol×K	1100.36	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=C837014&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