Benzene, 1,1'-thiobis[2-methyl-

Inchi: InChI=1S/C14H14S/c1-11-7-3-5-9-13(11)15-14-10-6-4-8-12(14)2/h3-10H,1-2H3
InchiKey: BDAJBOIAMYRWFR-UHFFFAOYSA-N
Formula: C14H14S
SMILES: Cc1ccccc1Sc1ccccc1C
Mol. weight [g/mol]: 214.33
CAS: 4537-05-7

Physical Properties

Property code	Value	Unit	Source
gf	305.68	kJ/mol	Joback Method
hf	159.70	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
ie	7.94	eV	NIST Webbook
log10ws	-4.84		Crippen Method
logp	4.455		Crippen Method
mcvol	176.950	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	651.82	K	Joback Method
tc	912.07	K	Joback Method
tf	359.82	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.68	J/mol×K	651.82	Joback Method
cpg	442.34	J/mol×K	695.19	Joback Method
cpg	457.65	J/mol×K	738.57	Joback Method
cpg	471.68	J/mol×K	781.94	Joback Method
cpg	484.49	J/mol×K	825.32	Joback Method
cpg	496.15	J/mol×K	868.69	Joback Method
cpg	506.72	J/mol×K	912.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4537057&Units=SI
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

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

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