2,2'-Thiobis(4-bromophenol)

Inchi: InChI=1S/C12H8Br2O2S/c13-7-1-3-9(15)11(5-7)17-12-6-8(14)2-4-10(12)16/h1-6,15-16H
InchiKey: HQRWNPFVXNLBJX-UHFFFAOYSA-N
Formula: C12H8Br2O2S
SMILES: Oc1ccc(Br)cc1Sc1cc(Br)ccc1O
Mol. weight [g/mol]: 376.06
CAS: 5336-22-1

Physical Properties

Property code	Value	Unit	Source
gf	8.24	kJ/mol	Joback Method
hf	-100.98	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.774		Crippen Method
mcvol	195.510	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	899.62	K	Joback Method
tc	1201.60	K	Joback Method
tf	680.32	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.75	J/mol×K	899.62	Joback Method
cpg	474.13	J/mol×K	949.95	Joback Method
cpg	484.92	J/mol×K	1000.28	Joback Method
cpg	496.45	J/mol×K	1050.61	Joback Method
cpg	509.06	J/mol×K	1100.94	Joback Method
cpg	523.08	J/mol×K	1151.27	Joback Method
cpg	538.86	J/mol×K	1201.60	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=C5336221&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