Benzene, 1,1'-thiobis[2,4,6-trinitro-

Other names:	Bis(2,4,6-trinitrophenyl)sulfide
	Picryl sulfide
	2,4,6-Trinitrophenyl sulfide
	2,4,6,2',4',6'-Hexanitrodiphenyl sulfide
	Dipicryl sulfide
	Dipicryl sulphide
	UN 0401
	NSC 243670
	bis(2,4,6-trinitrophenyl) sulphide
Inchi:	InChI=1S/C12H4N6O12S/c19-13(20)5-1-7(15(23)24)11(8(2-5)16(25)26)31-12-9(17(27)2
InchiKey:	XHJPTLWIOZRBQB-UHFFFAOYSA-N
Formula:	C12H4N6O12S
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Sc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c([N
Mol. weight [g/mol]:	456.26
CAS:	2217-06-3

Physical Properties

Property code	Value	Unit	Source
gf	463.62	kJ/mol	Joback Method
hf	90.54	kJ/mol	Joback Method
hfus	84.88	kJ/mol	Joback Method
hvap	157.19	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	3.287		Crippen Method
mcvol	253.290	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	1537.02	K	Joback Method
tc	1890.41	K	Joback Method
tf	1249.02	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	689.25	J/mol×K	1537.02	Joback Method
cpg	682.29	J/mol×K	1595.92	Joback Method
cpg	674.46	J/mol×K	1654.82	Joback Method
cpg	665.93	J/mol×K	1713.72	Joback Method
cpg	656.84	J/mol×K	1772.61	Joback Method
cpg	647.36	J/mol×K	1831.51	Joback Method
cpg	637.62	J/mol×K	1890.41	Joback Method

Sources

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=C2217063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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