1,3,7,9-Tetranitrophenothiazine,5-oxide

Inchi: InChI=1S/C12H5N5O9S/c18-14(19)5-1-7(16(22)23)11-9(3-5)27(26)10-4-6(15(20)21)2-8(
InchiKey: MACCEORDICAAII-UHFFFAOYSA-N
Formula: C12H5N5O9S
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2c(c1)S(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1N2
Mol. weight [g/mol]: 395.26
CAS: 27050-53-9

Physical Properties

Property code	Value	Unit	Source
chs	-5540.74	kJ/mol	NIST Webbook
gf	316.70	kJ/mol	Joback Method
hf	4.95	kJ/mol	Joback Method
hfs	-498.01	kJ/mol	NIST Webbook
hfus	74.06	kJ/mol	Joback Method
hvap	135.72	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	2.543		Crippen Method
mcvol	223.440	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	1257.58	K	Joback Method
tc	1572.83	K	Joback Method
tf	1143.66	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.45	J/mol×K	1257.58	Joback Method
cpg	662.11	J/mol×K	1310.12	Joback Method
cpg	668.91	J/mol×K	1362.66	Joback Method
cpg	676.06	J/mol×K	1415.20	Joback Method
cpg	683.74	J/mol×K	1467.74	Joback Method
cpg	692.16	J/mol×K	1520.29	Joback Method
cpg	701.51	J/mol×K	1572.83	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=C27050539&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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