Thioxanthene-3,7-diamine, 10,10-dioxide

Inchi: InChI=1S/C13H12N2O2S/c14-10-3-4-12-9(6-10)5-8-1-2-11(15)7-13(8)18(12,16)17/h1-4,
InchiKey: AVIIQKLBSWQNHI-UHFFFAOYSA-N
Formula: C13H12N2O2S
SMILES: Nc1ccc2c(c1)Cc1ccc(N)cc1S2(=O)=O
Mol. weight [g/mol]: 260.31
CAS: 116496-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.46	kJ/mol	Joback Method
hf	-167.55	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	90.69	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.588		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
tb	749.15	K	Joback Method
tc	998.82	K	Joback Method
tf	619.02	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.70	J/mol×K	749.15	Joback Method
cpg	504.89	J/mol×K	790.76	Joback Method
cpg	516.07	J/mol×K	832.37	Joback Method
cpg	526.34	J/mol×K	873.98	Joback Method
cpg	535.81	J/mol×K	915.60	Joback Method
cpg	544.59	J/mol×K	957.21	Joback Method
cpg	552.78	J/mol×K	998.82	Joback Method

Sources

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=C116496607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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