Thioxanthene

Other names:	9H-Thioxanthene
	Dibenzothiapyran
	Thiaxanthen
	Thiaxanthene
	Thioxanthen
	10H-dibenzo[b,e]thiin
Inchi:	InChI=1S/C13H10S/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-8H,9H2
InchiKey:	PQJUJGAVDBINPI-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	c1ccc2c(c1)Cc1ccccc1S2
Mol. weight [g/mol]:	198.28
CAS:	261-31-4

Physical Properties

Property code	Value	Unit	Source
gf	384.56	kJ/mol	Joback Method
hf	283.03	kJ/mol	Joback Method
hfus	19.55	kJ/mol	Joback Method
hsub	101.70 ± 1.60	kJ/mol	NIST Webbook
hsub	100.90 ± 0.20	kJ/mol	NIST Webbook
hvap	77.80 ± 2.60	kJ/mol	NIST Webbook
log10ws	-4.23		Crippen Method
logp	3.742		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	615.13	K	Joback Method
tc	884.01	K	Joback Method
tf	401.70 ± 0.10	K	NIST Webbook
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.25	J/mol×K	615.13	Joback Method

cpg	364.96	J/mol×K	659.94	Joback Method
cpg	378.32	J/mol×K	704.76	Joback Method
cpg	390.49	J/mol×K	749.57	Joback Method
cpg	401.65	J/mol×K	794.38	Joback Method
cpg	411.95	J/mol×K	839.20	Joback Method
cpg	421.57	J/mol×K	884.01	Joback Method
hfust	26.10	kJ/mol	401.80	NIST Webbook
hsubt	98.40 ± 0.20	kJ/mol	370.50	NIST Webbook
hvapt	69.50 ± 0.20	kJ/mol	415.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C261314&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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