Phenoxathiin

Other names:	1,4-Dibenzothioxine
	Dibenzooxathiane
	Dibenzothioxin
	NSC 464
	Phenothioxin
	Phenoxathiane
	Phenoxathine
	Phenoxathrin
	Phenoxthin
	RJC 03297
	USAF DO-17
Inchi:	InChI=1S/C12H8OS/c1-3-7-11-9(5-1)13-10-6-2-4-8-12(10)14-11/h1-8H
InchiKey:	GJSGGHOYGKMUPT-UHFFFAOYSA-N
Formula:	C12H8OS
SMILES:	c1ccc2c(c1)Oc1ccccc1S2
Mol. weight [g/mol]:	200.26
CAS:	262-20-4

Physical Properties

Property code	Value	Unit	Source
chs	-6498.70 ± 1.40	kJ/mol	NIST Webbook
gf	290.02	kJ/mol	Joback Method
hf	125.80 ± 1.00	kJ/mol	NIST Webbook
hfs	31.30 ± 1.70	kJ/mol	NIST Webbook
hfus	19.43	kJ/mol	Vapor Pressures of Solid and Liquid Xanthene and Phenoxathiin from Effusion and Static Studies
hvap	77.30 ± 0.10	kJ/mol	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	7.98 ± 0.03	eV	NIST Webbook
ie	7.72 ± 0.05	eV	NIST Webbook
log10ws	-3.77		Crippen Method
logp	3.944		Crippen Method
mcvol	143.780	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1651.00		NIST Webbook

ss	222.66	J/mol×K	NIST Webbook
tb	619.20	K	Joback Method
tc	890.04	K	Joback Method
tf	438.60	K	Joback Method
tt	328.77 ± 0.00	K	NIST Webbook
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.38	J/mol×K	709.48	Joback Method
cpg	393.41	J/mol×K	890.04	Joback Method
cpg	384.97	J/mol×K	844.90	Joback Method
cpg	375.92	J/mol×K	799.76	Joback Method
cpg	366.11	J/mol×K	754.62	Joback Method
cpg	330.49	J/mol×K	619.20	Joback Method
cpg	343.56	J/mol×K	664.34	Joback Method
cps	213.77	J/mol×K	298.15	NIST Webbook
hfust	20.27	kJ/mol	328.80	NIST Webbook
hfust	20.27	kJ/mol	328.80	NIST Webbook
hfust	19.43	kJ/mol	329.60	NIST Webbook
hfust	20.27	kJ/mol	328.78	NIST Webbook
hvapt	68.70	kJ/mol	502.50	NIST Webbook
hvapt	66.00	kJ/mol	502.50	NIST Webbook
hvapt	63.40	kJ/mol	502.50	NIST Webbook
hvapt	60.80	kJ/mol	502.50	NIST Webbook
hvapt	58.00	kJ/mol	502.50	NIST Webbook
hvapt	55.10	kJ/mol	502.50	NIST Webbook
psub	9.27e-04	kPa	324.50	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	7.71e-04	kPa	323.00	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	4.53e-04	kPa	318.20	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	2.17e-04	kPa	311.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	2.07e-04	kPa	311.50	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	
psub	2.09e-04	kPa	311.40	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique	

psub	1.43e-04	kPa	308.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	8.61e-05	kPa	304.20	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique:	https://www.doi.org/10.1016/j.jct.2010.01.014
Vapor Pressures of Solid and Liquid Xanthene and Phenoxathiin from Ebulliometry:	https://www.doi.org/10.1021/je800333q
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=C262204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume