Benzo(b)thiophene-2,3-dione

Other names:	Thioisatin
	Thianaphthenequinone
	Thionaphthenequinone
	Thionaphthoquinone
	2,3-Dioxo-2,3-dihydrothionaphthene
	2,3-Thionaphthenequinone
	Benzo[b]thiophen-2,3-dion
	2,3-Dihydrobenzo[b]thiophen-2,3-dione
	2,3-Dioxo-2,3-dihydrobenzo[b]thiophene
	Benzothiophene-2,3-dione
	NSC 114478
Inchi:	InChI=1S/C8H4O2S/c9-7-5-3-1-2-4-6(5)11-8(7)10/h1-4H
InchiKey:	MHESOLAAORBNPM-UHFFFAOYSA-N
Formula:	C8H4O2S
SMILES:	O=C1Sc2ccccc2C1=O
Mol. weight [g/mol]:	164.18
CAS:	493-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-120.39	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
ie	9.14 ± 0.05	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.502		Crippen Method
mcvol	108.450	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
tb	608.98	K	Joback Method
tc	888.41	K	Joback Method
tf	460.93	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.60	J/mol×K	608.98	Joback Method
cpg	249.98	J/mol×K	655.55	Joback Method
cpg	260.54	J/mol×K	702.12	Joback Method
cpg	270.26	J/mol×K	748.69	Joback Method
cpg	279.14	J/mol×K	795.27	Joback Method
cpg	287.18	J/mol×K	841.84	Joback Method
cpg	294.38	J/mol×K	888.41	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=C493572&Units=SI

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
ie: Ionization energy
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