2,3-DIOXO-2,3-DIHYDROBENZO[b]THIOPHENE/TH

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]:	164.19

Physical Properties

Property code	Value	Unit	Source
hf	-119.78	kJ/mol	Cheméo Relay (1.0)
hfus	9.87	kJ/mol	Joback Method
ie	9.14 ± 0.05	eV	NIST Webbook
log10ws	-3.12		Cheméo Relay (1.0)
logp	1.502		Crippen Method
mcvol	108.450	ml/mol	McGowan Method
tb	557.23	K	Cheméo Relay (1.0)
tf	418.75	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493572&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point