

9H-Thioxanthen-9-one

Other names:	10-Thioxanthone
	9-Thioxanthone
	9H-Thioxanthene, 9-oxo-
	NSC 15912
	NSC 658181
	Thiaxanthenone
	Thiaxanthon
	Thiaxanthone
	Thioxanthen-9-one
	Thioxanthene, 9-oxo-
	Thioxanthene-9-one
	Thioxanthenone
	thioxanthone
Inchi:	InChI=1S/C13H8OS/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8H
InchiKey:	YRHRIQCWCFGUEQ-UHFFFAOYSA-N
Formula:	C13H8OS
SMILES:	O=c1c2cccc2sc2cccc12
Mol. weight [g/mol]:	212.27

Physical Properties

Property code	Value	Unit	Source
chs	-6840.50 ± 3.50	kJ/mol	NIST Webbook
hf	94.30 ± 3.60	kJ/mol	NIST Webbook
hfs	-20.50 ± 3.60	kJ/mol	NIST Webbook
hfus	28.40	kJ/mol	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
hfus	106.50	kJ/mol	Experimental and Computational Studies on the Structural and Thermodynamic Properties of Two Sulfur Heterocyclic Keto Compounds
hsub	114.81 ± 0.41	kJ/mol	NIST Webbook
hsub	114.80 ± 0.40	kJ/mol	NIST Webbook
hvap	99.28	kJ/mol	Cheméo Relay (1.0)
ie	7.90	eV	Cheméo Relay (1.0)

log10ws	-5.54		Aqueous Solubility Prediction Method
logp	3.415		Crippen Method
mcvol	153.570	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
rinpol	346.20		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	657.01	K	Cheméo Relay (1.0)
tf	487.88 ± 0.02	K	NIST Webbook
tf	482.00	K	Solubilities of Some Thioxanthone Derivatives in Supercritical CO2

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.50	kJ/mol	487.88	NIST Webbook
hfust	35.50	kJ/mol	487.90	NIST Webbook
hfust	35.50	kJ/mol	487.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	645.20	K	95.30	NIST Webbook

Sources

Solubilities of Some Thioxanthone Derivatives in Supercritical CO₂: Experimental and Computational Studies on the Structural and Thermodynamic Properties of Aromatic Solids in Pressurized Hot Water: Cheméo Relay (1.0):

<https://www.doi.org/10.1021/je020163y>

<https://www.doi.org/10.1021/je100603q>

<https://www.doi.org/10.1021/je800707x>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C492228&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Thermodynamic Study on the Sublimation of Anthracene-Like Compounds:

<https://www.doi.org/10.1021/je100850z>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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