Xanthone

Other names:	9-Xanthenone
	9-Xanthone
	9-oxoxanthene
	9H-Xanthene, 9-oxo-
	9H-xanthen-9-one
	Benzophenone oxide
	Dibenzo-«gamma»-pyrone
	Diphenylene ketone oxide
	E 6
	Genicide
	NSC 14978
	Xanthen-9-one
	Xanthene, 9-oxo-
	Xanthenone
	dibenzopyranone
Inchi:	InChI=1S/C13H8O2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8H
InchiKey:	JNELGWHKGNBSMD-UHFFFAOYSA-N
Formula:	C13H8O2
SMILES:	O=c1c2ccccc2oc2ccccc12
Mol. weight [g/mol]:	196.20
CAS:	90-47-1

Physical Properties

Property code	Value	Unit	Source
chs	-6062.20 ± 3.60	kJ/mol	NIST Webbook
chs	-6067.00 ± 2.00	kJ/mol	NIST Webbook
hf	-98.20 ± 3.60	kJ/mol	NIST Webbook
hf	-92.90	kJ/mol	NIST Webbook
hfs	-196.80 ± 3.60	kJ/mol	NIST Webbook
hfs	-191.50 ± 2.70	kJ/mol	NIST Webbook
hfus	26.60	kJ/mol	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
hsub	102.70 ± 2.30	kJ/mol	NIST Webbook
hsub	98.57 ± 0.36	kJ/mol	NIST Webbook
hsub	98.60	kJ/mol	NIST Webbook
hsub	98.60 ± 0.40	kJ/mol	NIST Webbook

hsub	112.00 ± 6.30	kJ/mol	NIST Webbook
ie	8.42 ± 0.03	eV	NIST Webbook
log10ws	-8.24		Crippen Method
logp	2.946		Crippen Method
mcvol	143.090	ml/mol	McGowan Method
rinpol	1775.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	328.31		NIST Webbook
rinpol	313.00		NIST Webbook
rinpol	313.10		NIST Webbook
rinpol	313.05		NIST Webbook
rinpol	326.50		NIST Webbook
rinpol	325.80		NIST Webbook
rinpol	312.30		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tt	448.80	K	Thermodynamic properties of xanthone: Heat capacities, phase-transition properties, and thermodynamic-consistency analyses using computational results

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	226.00	J/mol×K	298.15	NIST Webbook
hfust	26.12	kJ/mol	449.63	NIST Webbook
hfust	26.12	kJ/mol	449.70	NIST Webbook
hvapt	98.57	kJ/mol	298.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	622.70	K	97.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of xanthone and xanthene in supercritical CO2:	https://www.doi.org/10.1016/j.fluid.2005.09.008
Thermodynamic properties of xanthone: Heat capacities, phase transition properties, and thermodynamic consistency analyses using computational results:	https://www.doi.org/10.1016/j.jct.2015.02.009
Thermodynamic Study on the Sublimation of Anthracene-Like Solids:	https://www.doi.org/10.1021/je100850z
Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water:	https://www.doi.org/10.1021/je800707x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90471&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
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
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
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure
tt:	Triple Point Temperature