9H-Xanthene

Other names:	10H-9-oxaanthracene
	9-H-Xathene
	Dibenzo[a,e]pyran
	Dibenzopyran, tricyclic
	NSC 46931
	dibenzopyran
	xanthene
Inchi:	InChI=1S/C13H10O/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-8H,9H2
InchiKey:	GJCOSYZMQJWQCA-UHFFFAOYSA-N
Formula:	C13H10O
SMILES:	c1ccc2c(c1)Cc1ccccc1O2
Mol. weight [g/mol]:	182.22
CAS:	92-83-1

Physical Properties

Property code	Value	Unit	Source
gf	258.58	kJ/mol	Joback Method
hf	105.77	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Vapor Pressures of Solid and Liquid Xanthene and Phenoxathiin from Effusion and Static Studies
hvap	54.97	kJ/mol	Joback Method
ie	7.65 ± 0.02	eV	NIST Webbook
log10ws	-3.45		Crippen Method
logp	3.383		Crippen Method
mcvol	141.520	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1645.80		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	281.80		NIST Webbook
rinpol	279.10		NIST Webbook
rinpol	281.04		NIST Webbook

rinpol	280.48		NIST Webbook
rinpol	1645.80		NIST Webbook
rinpol	281.80		NIST Webbook
rinpol	1659.80		NIST Webbook
tb	584.20	K	NIST Webbook
tc	847.39	K	Joback Method
tf	373.70 ± 0.10	K	NIST Webbook
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.54	J/mol×K	636.44	Joback Method
cpg	363.91	J/mol×K	678.63	Joback Method
cpg	376.14	J/mol×K	720.82	Joback Method
cpg	387.36	J/mol×K	763.01	Joback Method
cpg	397.69	J/mol×K	805.20	Joback Method
cpg	407.26	J/mol×K	847.39	Joback Method
cpg	335.88	J/mol×K	594.25	Joback Method
dvisc	0.0013082	Pa×s	404.39	Joback Method
dvisc	0.0010046	Pa×s	442.36	Joback Method
dvisc	0.0008043	Pa×s	480.34	Joback Method
dvisc	0.0006653	Pa×s	518.31	Joback Method
dvisc	0.0005647	Pa×s	556.28	Joback Method
dvisc	0.0017995	Pa×s	366.42	Joback Method
dvisc	0.0004895	Pa×s	594.25	Joback Method
hfust	19.20	kJ/mol	373.70	NIST Webbook
hfust	19.20	kJ/mol	373.70	NIST Webbook
hfust	15.87	kJ/mol	374.30	NIST Webbook
hfust	20.67	kJ/mol	374.60	NIST Webbook
hsubt	92.50	kJ/mol	329.00	NIST Webbook
hvapt	54.40	kJ/mol	506.50	NIST Webbook
hvapt	92.00	kJ/mol	298.15	Energetic effects of ether and ketone functional groups in 9,10-dihydroanthracene compound
hvapt	56.70	kJ/mol	506.50	NIST Webbook
hvapt	59.20	kJ/mol	506.50	NIST Webbook
hvapt	61.10	kJ/mol	506.50	NIST Webbook
hvapt	64.50	kJ/mol	506.50	NIST Webbook
hvapt	88.70	kJ/mol	423.00	NIST Webbook

Sources

Solubilities of xanthone and xanthene in supercritical CO2:	https://www.doi.org/10.1016/j.fluid.2005.09.008
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 9-fluorenone, thianthrene and xanthene in organic solvents:	https://www.doi.org/10.1016/j.fluid.2005.02.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92831&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Energetic effects of ether and ketone functional groups in 9,10-dihydroanthracene compounds:	https://www.doi.org/10.1016/j.jct.2010.04.027
Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water:	https://www.doi.org/10.1021/je800707x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor Pressures of Solid and Liquid Xanthene and Phenoxathiin from Effusion and Static Studies:	https://www.doi.org/10.1021/je800333q

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume