9,10-Anthracenedione, 1,4-dihydroxy-

Other names:	Anthraquinone, 1,4-dihydroxy-
	C.I. 58050
	Chinizarin
	Quinizarin
	Quinizarine
	Smoke Orange R
	1,4-Dihydroxy-9,10-anthraquinone
	1,4-Dihydroxyanthraquinone
	Macrolex Orange GG
	Solvent Orange 86
	1,4-Dihydroxyanthrachinon
	1,4-Dioxyanthraquinone
	1,4-Doa
	1,4-Dihydroxy-9,10-anthracenedione
	NSC 15367
	NSC 646569
Inchi:	InChI=1S/C14H8O4/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-6,15-16H
InchiKey:	GUEIZVNYDFNHJU-UHFFFAOYSA-N
Formula:	C14H8O4
SMILES:	O=C1c2ccccc2C(=O)c2c(O)ccc(O)c21
Mol. weight [g/mol]:	240.21
CAS:	81-64-1

Physical Properties

Property code	Value	Unit	Source
chs	-6057.40 ± 1.00	kJ/mol	NIST Webbook
gf	-201.30	kJ/mol	Joback Method
hf	-471.00 ± 2.30	kJ/mol	NIST Webbook
hfs	-595.10 ± 1.40	kJ/mol	NIST Webbook
hfus	29.07	kJ/mol	Joback Method
hsub	124.10 ± 0.90	kJ/mol	NIST Webbook
hsub	124.10	kJ/mol	NIST Webbook
hvap	87.21	kJ/mol	Joback Method
ie	7.94 ± 0.03	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	1.873		Crippen Method
mcvol	164.620	ml/mol	McGowan Method

pc	4931.51	kPa	Joback Method
rinpol	366.00		NIST Webbook
rinpol	365.29		NIST Webbook
rinpol	360.00		NIST Webbook
rinpol	360.00		NIST Webbook
tb	887.06	K	Joback Method
tc	1170.41	K	Joback Method
tf	472.71 ± 0.35	K	NIST Webbook
tf	472.95 ± 0.25	K	NIST Webbook
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.27	J/mol×K	1170.41	Joback Method
cpg	484.36	J/mol×K	887.06	Joback Method
cpg	496.32	J/mol×K	934.29	Joback Method
cpg	508.20	J/mol×K	981.51	Joback Method
cpg	520.20	J/mol×K	1028.74	Joback Method
cpg	532.57	J/mol×K	1075.96	Joback Method
cpg	545.52	J/mol×K	1123.19	Joback Method
hsubt	123.50	kJ/mol	376.00	NIST Webbook
hsubt	89.10	kJ/mol	513.00	NIST Webbook
hsubt	115.30	kJ/mol	363.00	NIST Webbook
hsubt	103.50 ± 1.30	kJ/mol	409.00	NIST Webbook
hsubt	102.40 ± 4.40	kJ/mol	363.00	NIST Webbook
hsubt	121.90 ± 0.80	kJ/mol	428.50	NIST Webbook
hsubt	121.00 ± 4.00	kJ/mol	429.00	NIST Webbook
hvapt	74.00	kJ/mol	551.00	NIST Webbook

Sources

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=C81641&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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