9,10-Anthracenedione, 1,5-dihydroxy-

Other names:	Anthraquinone, 1,5-dihydroxy-
	Anthrarufin
	1,5-Dihydroxyanthraquinone
	1,5-Dihydroxy-9,10-anthraquinone
	1,5-Dihydroxyanthrachinon
	1,5-Dihydroxy-9,10-anthracenedione
Inchi:	InChI=1S/C14H8O4/c15-9-5-1-3-7-11(9)14(18)8-4-2-6-10(16)12(8)13(7)17/h1-6,15-16H
InchiKey:	JPICKYUTICNNNJ-UHFFFAOYSA-N
Formula:	C14H8O4
SMILES:	O=C1c2cccc(O)c2C(=O)c2cccc(O)c21
Mol. weight [g/mol]:	240.21
CAS:	117-12-4

Physical Properties

Property code	Value	Unit	Source
gf	-201.30	kJ/mol	Joback Method
hf	-412.89	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hsub	117.60	kJ/mol	NIST Webbook
hvap	87.21	kJ/mol	Joback Method
ie	8.53 ± 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
tb	887.06	K	Joback Method
tc	1170.41	K	Joback Method
tf	711.00	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	559.27	J/mol×K	1170.41	Joback Method
hsubt	111.30	kJ/mol	456.00	NIST Webbook
hsubt	126.80	kJ/mol	398.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume