

9,10-Anthracenedione, 1-hydroxy-

Other names:	Anthraquinone, 1-hydroxy- «alpha»-Hydroxyanthraquinone 1-Hydroxyanthraquinone 1-Hydroxy-9,10-anthraquinone 1-Hydroxyanthrachinon
Inchi:	InChI=1S/C14H8O3/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7,15H
InchiKey:	BTLXPCBPYBNQNR-UHFFFAOYSA-N
Formula:	C14H8O3
SMILES:	O=C1c2ccccc2C(=O)c2c(O)cccc21
Mol. weight [g/mol]:	224.21
CAS:	129-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-46.68	kJ/mol	Joback Method
hf	-235.58	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
ie	8.43 ± 0.05	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	2.168		Crippen Method
mcvol	158.750	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	806.44	K	Joback Method
tc	1086.28	K	Joback Method
tf	599.28	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.96	J/mol×K	993.00	Joback Method
cpg	498.73	J/mol×K	1039.64	Joback Method
cpg	444.26	J/mol×K	806.44	Joback Method

cpg	456.54	J/mol×K	853.08	Joback Method
cpg	468.00	J/mol×K	899.72	Joback Method
cpg	478.76	J/mol×K	946.36	Joback Method
cpg	508.22	J/mol×K	1086.28	Joback Method
hsubt	101.30 ± 0.40	kJ/mol	407.00	NIST Webbook
hsubt	120.60	kJ/mol	358.00	NIST Webbook

Sources

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=C129431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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