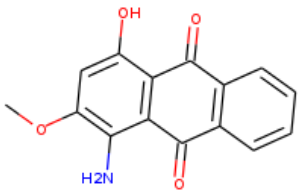
Anthraquinone, 1-amino-4-hydroxy-2-methoxy-



Other names: 1-Amino-2-methoxy-4-oxyanthraquinone; 1-Amino-4-hydroxy-2-methoxy-9,10-anthracenedione; 1-Amino-4-hydroxy-2-methoxyanthraquinone; 1a-2Mo-4oa; Acetoquinone Light Pink RLZ; Anthraquinone, 1-amino-4-hydroxy-2-methoxy-; Artisil Brilliant Pink RFS; C.I. 60755; C.I. Disperse Red 4; Celliton Fast Pink RF; Celliton Fast Pink RFA-CF; Cerven disperzni 4; Cilla Fast Pink RF; Dianix Fast Pink R; Disperse Pink Zh; Disperse Red-4; Disperse Rose Zh; Esteroquinone Light Pink RLL; Fenacet Fast Pink RF; Interchem Acetate Fast Pink DNA; Miketon Fast Pink RL; Miketon Polyester Pink RL; NSC 81265; Nyloquinone Pink B; Palanil Pink RF; Perliton Brilliant Pink R; Samaron Pink RFL; Supracet Fast Pink 2R.

InChI: InChI=1S/C15H11NO4/c1-20-10-6-9(17)11-12(13(10)16)15(19)8-5-3-2-4-7(8)14(11)18/h2-6,17H,16H2,1H3

InChI Key: WSPPHHAIMCTKNN-UHFFFAOYSA-N

Formula: C15H11NO4

SMILES: COc1cc(O)c2c(c1N)C(=O)c1ccccc1C2=O

Molecular Weight: 269.25

CAS: 2379-90-0

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-96.07	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-377.59	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.48	kJ/mol	Joback Method
$\Delta_{vap} H°$	90.79	kJ/mol	Joback Method
$log P_{oct/wat}$	1.76		Crippen Method
P_c	3633.35	kPa	Joback Method
T_{boil}	934.23	K	Joback Method
T_c	1206.05	K	Joback Method
T_{fus}	741.08	K	Joback Method
V_c	0.65	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	574.01	J/mol×K	934.23	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H11NO4/c1-20-10-6-9(17)11-12(13(10)16)15(19)8-5-3-2-4-7(8)14(11)18/h2-6,17H,16H2,1H3

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°$_{gas}$**: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).