

3-Nitroalizarine

Other names: 1,2-dihydroxy-3-nitroanthraquinone.

InChI: InChI=1S/C14H7NO6/c16-11-6-3-1-2-4-7(6)12(17)10-8(11)5-9(15(20)21)13(18)14(10)19/h1-5,18-19H

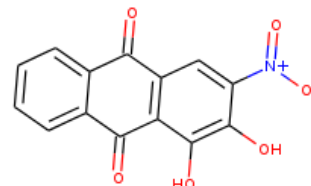
InChI Key: XZSUEVFAMOKROK-UHFFFAOYSA-N

Formula: C₁₄H₇NO₆

SMILES: O=C1c2ccccc2C(=O)c2c(O)c(O)c([N+](=O)[O-])cc21

Molecular Weight: 285.21

CAS: 568-93-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-175.38	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-435.12	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	40.04	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	104.46	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.78		Crippen Method
P_c	4910.80	kPa	Joback Method
T_{boil}	1043.88	K	Joback Method
T_c	1339.00	K	Joback Method
T_{fus}	867.13	K	Joback Method
V_c	0.60	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	567.34	J/mol×K	1043.88	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H7NO6/c16-11-6-3-1-2-4-7\(6\)12\(17\)10-8\(11\)5-9\(15\(20\)21\)13\(18\)14\(10\)19/h1-5,18-19H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H7NO6/c16-11-6-3-1-2-4-7(6)12(17)10-8(11)5-9(15(20)21)13(18)14(10)19/h1-5,18-19H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: 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 (m³/kg-mol).

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