

Anhalonine

Other names: Anhalonine.

InChI: InChI=1S/C12H15NO3/c1-7-10-8(3-4-13-7)5-9(14-2)11-12(10)16-6-15-11/h5,7,13H,3-4,6H2,1-2H3

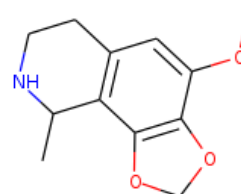
InChI Key: YEGBVDVRKMCCON-UHFFFAOYSA-N

Formula: C₁₂H₁₅NO₃

SMILES: COc1cc2c(c3c1OCO3)C(C)NCC2

Molecular Weight: 221.25

CAS: 519-04-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	51.63	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-298.99	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.16	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	65.73	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.63		Crippen Method
P_c	3117.52	kPa	Joback Method
T_{boil}	667.85	K	Joback Method
T_c	906.52	K	Joback Method
T_{fus}	518.50	K	Joback Method
V_c	0.60	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	448.85	J/mol×K	667.85	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15NO3/c1-7-10-8\(3-4-13-7\)5-9\(14-2\)11-12\(10\)16-6-15-11/h5,7,13H,3-4,6H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15NO3/c1-7-10-8(3-4-13-7)5-9(14-2)11-12(10)16-6-15-11/h5,7,13H,3-4,6H2,1-2H3)

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

Legend

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

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

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

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

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

$logP_{oct/wat}$: 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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