

Antazoline, hydrolized, acetylated

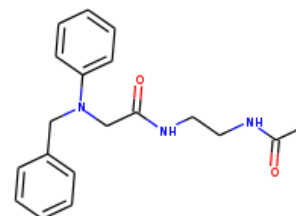
InChI: InChI=1S/C19H23N3O2/c1-16(23)20-12-13-21-19(24)15-22(18-10-6-3-7-11-18)14-17-8-4-2-5-9-17/h2-11H,12-15H2,1H3,(H,20,23)(H,21,24)

InChI Key: QJYCWNIEOSWHAH-UHFFFAOYSA-N

Formula: C19H23N3O2

SMILES: CC(=O)NCCNC(=O)CN(Cc1ccccc1)c1ccccc1

Molecular Weight: 325.40



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	365.64	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-13.12	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	49.46	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	90.85	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.945		Crippen Method
P_c	2010.90	kPa	Joback Method
T_{boil}	908.00	K	Joback Method
T_c	1135.24	K	Joback Method
T_{fus}	594.38	K	Joback Method
V_c	0.984	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	821.69	J/mol×K	908.0	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H23N3O2/c1-16\(23\)20-12-13-21-19\(24\)15-22\(18-10-6-3-7-11-18\)14-17-8-4-2-5-9-17/h2-11H,12-15H2,1H3,\(H,20,23\)\(H,21,24\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H23N3O2/c1-16(23)20-12-13-21-19(24)15-22(18-10-6-3-7-11-18)14-17-8-4-2-5-9-17/h2-11H,12-15H2,1H3,(H,20,23)(H,21,24))

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

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).

$\log P_{oct/wat}$: 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 (m³/kg-mol).

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