

Oxprenolol hydroxy - H2O, isomer II, acetylated

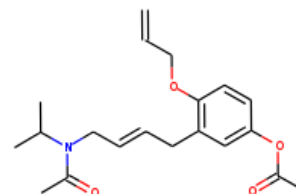
InChI: InChI=1S/C20H27NO4/c1-6-13-24-20-11-10-19(25-17(5)23)14-18(20)9-7-8-12-21(15(2)3)16(4)22/h6-8,10-11,14-15H,1,9,12-13H2,2-5H3/b8-7+

InChI Key: ZELDAZQWTKTVKR-BQYQJAHWSA-N

Formula: C20H27NO4

SMILES: C=CCOc1ccc(OC(C)=O)cc1CC=CCN(C(C)=O)C(C)C

Molecular Weight: 345.43



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	19.23	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-427.24	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	44.81	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	82.97	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.53		Crippen Method
P_c	1429.38	kPa	Joback Method
T_{boil}	859.06	K	Joback Method
T_c	1067.25	K	Joback Method
T_{fus}	521.57	K	Joback Method
V_c	1.07	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	865.63	J/mol×K	859.06	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H27NO4/c1-6-13-24-20-11-10-19\(25-17\(5\)23\)14-18\(20\)9-7-8-12-21\(15\(2\)3\)16\(4\)22/h6-8,10-11,14-15H,1,9,12-13H2,2-5H3/b8-7+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H27NO4/c1-6-13-24-20-11-10-19(25-17(5)23)14-18(20)9-7-8-12-21(15(2)3)16(4)22/h6-8,10-11,14-15H,1,9,12-13H2,2-5H3/b8-7+)

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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