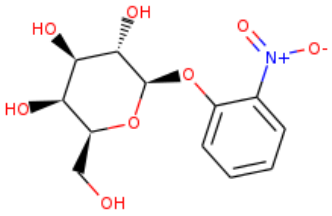
o-Nitrophenyl-«beta»-D-galactopyranoside

Other names: 2-Nitrophenyl-«beta»-D-galactopyranoside; 2-Nitrophenyl-«beta»-«delta»-galactopyranoside; 2-nitrophenyl-beta-D-galactopyranoside; Galactopyranoside, o-nitrophenyl, beta-D-; Galactopyranoside, o-nitrophenyl, «beta»-D-; o-Nitrophenyl «beta»-D-galactoside; o-Nitrophenyl «beta»-galactoside; «beta»-D-Galactopyranoside, 2-nitrophenyl.



InChI: InChI=1S/C12H15NO8/c14-5-8-9(15)10(16)11(17)12(21-8)20-7-4-2-1-3-6(7)13(18)19/h1-4,8-12,14-17H,5H2/t8-,9+,10+,11-,12-/m0/s1

InChI Key: KUWPCJHYPSUOFW-KNZXXDILSA-N

Formula: C12H15NO8

SMILES: O=[N+]([O-])c1ccccc1OC1OC(CO)C(O)C(O)C1O

Molecular Weight: 301.25

CAS: 369-07-3

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-556.30	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-976.89	kJ/mol	Joback Method
$\Delta_{fus} H°$	53.49	kJ/mol	Joback Method
$\Delta_{vap} H°$	134.66	kJ/mol	Joback Method
$logP_{oct/wat}$	-1.23		Crippen Method
P_c	3777.68	kPa	Joback Method
T_{boil}	1076.42	K	Joback Method
T_c	1318.89	K	Joback Method
T_{fus}	690.05	K	Joback Method
V_c	0.73	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	700.82	J/mol×K	1076.42	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15NO8/c14-5-8-9(15)10(16)11(17)12(21-8)20-7-4-2-1-3-6(7)13(18)19/h1-4,8-12,14-17H,5H2/t8-,9+,10+,11-,12-/m0/s1
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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