

o-Nitrophenyl-«beta»-D-galactopyranoside

Other names:	2-Nitrophenyl-«beta»-D-galactopyranoside 2-Nitrophenyl-«beta»-«delta»-galactopyranoside «beta»-D-Galactopyranoside, 2-nitrophenyl o-Nitrophenyl «beta»-galactoside o-Nitrophenyl «beta»-D-galactoside Galactopyranoside, o-nitrophenyl, «beta»-D- Galactopyranoside, o-nitrophenyl, beta-D- 2-nitrophenyl-beta-D-galactopyranoside
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
InchiKey:	KUWPCJHYPSUOFW-KNZXXDILSA-N
Formula:	C12H15NO8
SMILES:	O=[N+]([O-])c1ccccc1OC1OC(CO)C(O)C(O)C1O
Mol. weight [g/mol]:	301.25
CAS:	369-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-556.30	kJ/mol	Joback Method
hf	-976.89	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	134.66	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	-1.227		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	1076.42	K	Joback Method
tc	1318.89	K	Joback Method
tf	690.05	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.82	J/mol×K	1076.42	Joback Method

cpg	705.74	J/mol×K	1116.83	Joback Method
cpg	709.21	J/mol×K	1157.24	Joback Method
cpg	711.23	J/mol×K	1197.66	Joback Method
cpg	711.81	J/mol×K	1238.07	Joback Method
cpg	710.97	J/mol×K	1278.48	Joback Method
cpg	708.71	J/mol×K	1318.89	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C369073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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