

1,3-Propanediol, 2-amino-1-(4-nitrophenyl)-

Other names:

1-(p-Nitrophenyl)-2-amino-1,3-propanediol
1,3-Propanediol, 2-amino-1-(p-nitrophenyl)-
Phenylpropanol, «alpha»-amino-«beta»-hydroxy-4-nitro-
2-amino-1-(4-nitrophenyl)propane-1,3-diol

Inchi:

InChI=1S/C9H12N2O4/c10-8(5-12)9(13)6-1-3-7(4-2-6)11(14)15/h1-4,8-9,12-13H,5,10H2

InchiKey:

OCYJXSUPZMNXEN-UHFFFAOYSA-N

Formula:

C9H12N2O4

SMILES:

NC(CO)C(O)c1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]:

212.20

CAS:

119-62-0

Physical Properties

Property code	Value	Unit	Source
chs	-4934.36	kJ/mol	NIST Webbook
gf	-48.84	kJ/mol	Joback Method
hf	-296.02	kJ/mol	Joback Method
hfus	30.41	kJ/mol	Joback Method
hvap	98.38	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	-0.052		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
tb	844.83	K	Joback Method
tc	1064.91	K	Joback Method
tf	548.64	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.77	J/molxK	844.83	Joback Method
cpg	460.81	J/molxK	881.51	Joback Method
cpg	468.22	J/molxK	918.19	Joback Method
cpg	475.04	J/molxK	954.87	Joback Method

cpg	481.33	J/mol×K	991.55	Joback Method
cpg	487.11	J/mol×K	1028.23	Joback Method
cpg	492.44	J/mol×K	1064.91	Joback Method

Sources

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=C119620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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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