4-Hydroxy-3-nitrophenylacetic acid

Other names:	3-Nitro-4-hydroxy phenylacetic acid
	Benzeneacetic acid, 4-hydroxy-3-nitro-
Inchi:	InChI=1S/C8H7NO5/c10-7-2-1-5(4-8(11)12)3-6(7)9(13)14/h1-3,10H,4H2,(H,11,12)
InchiKey:	QBHBHOSRLDPIHG-UHFFFAOYSA-N
Formula:	C8H7NO5
SMILES:	O=C(O)Cc1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	197.14
CAS:	10463-20-4

Physical Properties

Property code	Value	Unit	Source
gf	-265.55	kJ/mol	Joback Method
hf	-436.27	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.927		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	792.61	K	Joback Method
tc	1029.34	K	Joback Method
tf	584.94	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.02	J/mol×K	792.61	Joback Method
cpg	359.28	J/mol×K	832.06	Joback Method
cpg	366.15	J/mol×K	871.52	Joback Method
cpg	372.71	J/mol×K	910.97	Joback Method
cpg	379.05	J/mol×K	950.43	Joback Method
cpg	385.25	J/mol×K	989.88	Joback Method
cpg	391.41	J/mol×K	1029.34	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=C10463204&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