Levodopa

Other names:

(-)-(3,4-Dihydroxyphenyl)alanine
(-)-Dopa
3,4-Dihydroxy-L-phenylalanine
3,4-Dihydroxyphenyl-L-alanine
3,4-Dihydroxyphenylalanine
3-(3,4-Dihydroxyphenyl)-L-Alanine
3-Hydroxy-L-tyrosine
Alanine, 3-(3,4-dihydroxyphenyl)-, (-)-
Alanine, 3-(3,4-dihydroxyphenyl)-, L-
Bendopa
Brocadopa
Cidandopa
DA
DOPA
Deadopa
Dihydroxy-L-phenylalanine
Dopaflex
Dopaidan
Dopal
Dopal-Fher
Dopalina
Dopar
Doparkine
Doparl
Dopasol
Dopaston
Dopaston SE
Dopastral
Doprin
Eldopal
Eldopar
Eldopatec
Eurodopa
Helfo-Dopa
Insulamina
L-(-)-Dopa
L-(3,4-Dihydroxyphenyl)-«alpha»-alanine
L-(3,4-Dihydroxyphenyl)alanine
L-(o-Dihydroxyphenyl)alanine
L-3,4-dihydroxyphenylalanine

	L-3-(3,4-Dihydroxyphenyl)alanine
	L-3-hydroxytyrosine
	L-DOPA
	L-Tyrosine, 3-hydroxy-
	L-o-Hydroxytyrosine
	L-«beta»-(3,4-Dihydroxyphenyl)alanine
	Larodopa
	Ledopa
	Levedopa
	Levopa
	Maipedopa
	Parda
	Pardopa
	Prodopa
	Ro 4-6316
	Syndopa
	Veldopa
	Weldopa
	«beta»-(3,4-Dihydroxyphenyl)-L-alanine
	«beta»-(3,4-Dihydroxyphenyl)alanine
Inchi:	InChI=1S/C9H11NO4/c10-6(9(13)14)3-5-1-2-7(11)8(12)4-5/h1-2,4,6,11-12H,3,10H2,(H,1
InchiKey:	WTDRDQBEARUVNC-LURJTMIESA-N
Formula:	C9H11NO4
SMILES:	NC(Cc1ccc(O)c(O)c1)C(=O)O
Mol. weight [g/mol]:	197.19
CAS:	59-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-373.66	kJ/mol	Joback Method
hf	-583.48	kJ/mol	Joback Method
hfus	32.03	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.052		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	6577.70	kPa	Joback Method
tb	811.38	K	Joback Method
tc	1042.02	K	Joback Method

tf	550.15	K	Low-Temperature Heat Capacities and Standard Molar Enthalpy of Formation of L-3-(3,4-Dihydroxyphenyl) Alanine (C9H11NO4)
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.91	J/mol×K	811.38	Joback Method
cpg	422.15	J/mol×K	849.82	Joback Method
cpg	430.24	J/mol×K	888.26	Joback Method
cpg	438.32	J/mol×K	926.70	Joback Method
cpg	446.51	J/mol×K	965.14	Joback Method
cpg	454.96	J/mol×K	1003.58	Joback Method
cpg	463.81	J/mol×K	1042.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Diffusion of levodopa in aqueous solutions of hydrochloric acid at 25 C:	https://www.doi.org/10.1016/j.jct.2013.12.010
Low-Temperature Heat Capacities and Standard Molar Enthalpy of Formation of L-3-(3,4-Dihydroxyphenyl) Alanine (C9H11NO4):	https://www.doi.org/10.1021/je700644s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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