Dihydroxyphenylalanine

Other names: 3(3,4-Dihydroxyphenyl)-dl-alanine
dl-3,4-Dihydroxyphenylalanine
dl-Dopa
dl-«beta»-(3,4-Dihydroxyphenyl)-«alpha»-alanine
DL-Tyrosine, 3-hydroxy-
«beta»-(3,4-Dihydroxyphenyl)-DL-«alpha»-alanine
(.+/-.)-Dopa
(.+/-.)-3-(3,4-Dihydroxyphenyl)alanine
(.+/-.)-3,4-Dihydroxyphenylalanine
Alanine, 3-(3,4-dihydroxyphenyl)-, DL-
DL-«beta»-(3,4-Dihydroxyphenyl)alanine
DL-Dihydroxyphenylalanine
DL-Dioxyphenylalanine
DL-3,4-DOPA
3,4-Dihydroxy-DL-phenylalanine
3',4'-Dihydroxyphenylalanine
(R,S)-Dopa
NSC 16940

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-UHFFFAOYSA-N

Formula: C9H11NO4

SMILES: NC(Cc1ccc(O)c(O)c1)C(=O)O

Mol. weight [g/mol]: 197.19

CAS: 63-84-3

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	620.06	K	Joback Method
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

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=C63843&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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