Tyrosine

Other names:	(-)-«alpha»-Amino-p-hydroxyhydrocinnamic acid (S)-Tyrosine (S)-«alpha»-Amino-4-hydroxybenzenepropanoic acid 3-(p-hydroxyphenyl)-L-alanine 4-HYDROXY-L-PHENYLALANINE Benzenepropanoic acid, «alpha»-amino-4-hydroxy-, (S)- L-2-Amino-3-p-hydroxyphenylpropanoic acid L-Phenylalanine, 4-hydroxy- L-TYROSINE L-p-Tyrosine NSC 82624 P-TYROSINE Propanoic acid, 2-amino-3-(4-hydroxyphenyl)-, (S)- Tyrosine, L- «alpha»-Amino-«beta»-(4-hydroxyphenyl)propionic acid
Inchi:	InChI=1S/C9H11NO3/c10-8(9(12)13)5-6-1-3-7(11)4-2-6/h1-4,8,11H,5,10H2,(H,12,13)/t8-
InchiKey:	OUYCCCASQSFEME-MRVPVSSYSA-N
Formula:	C9H11NO3
SMILES:	NC(Cc1ccc(O)cc1)C(=O)O
Mol. weight [g/mol]:	181.19
CAS:	60-18-4

Physical Properties

Property code	Value	Unit	Source
affp	926.00	kJ/mol	NIST Webbook
basg	892.10	kJ/mol	NIST Webbook
chs	-4481.70	kJ/mol	NIST Webbook
chs	-4428.10 ± 1.50	kJ/mol	NIST Webbook
gf	-219.04	kJ/mol	Joback Method
hf	-406.17	kJ/mol	Joback Method
hfs	-685.60 ± 1.50	kJ/mol	NIST Webbook
hfus	26.25	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.347		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method

ss	214.01	J/mol×K	NIST Webbook
ss	221.80	J/mol×K	NIST Webbook
tb	730.76	K	Joback Method
tc	953.99	K	Joback Method
tf	508.34	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.44	J/mol×K	730.76	Joback Method
cpg	385.36	J/mol×K	767.97	Joback Method
cpg	393.72	J/mol×K	805.17	Joback Method
cpg	401.61	J/mol×K	842.38	Joback Method
cpg	409.12	J/mol×K	879.58	Joback Method
cpg	416.32	J/mol×K	916.79	Joback Method
cpg	423.30	J/mol×K	953.99	Joback Method
cps	216.44	J/mol×K	298.15	NIST Webbook
cps	214.30	J/mol×K	294.60	NIST Webbook
hsubt	101.00 ± 8.00	kJ/mol	462.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60184&Units=SI

Solubility of d-Tryptophan and l-Tyrosine in Several Organic Solvents: Determination and Solvent Effect: https://www.doi.org/10.1021/acs.jced.9b00258

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Solubility of l-tyrosine in aqueous solutions of methanol, ethanol, 1-propanol and dimethyl sulfoxide: Experimental determination and preferential solvation analysis: https://www.doi.org/10.1016/j.jct.2018.05.011

Volumetric and acoustic studies of l-tyrosine + l-glutamic acid + water at different temperatures: https://www.doi.org/10.1016/j.tca.2014.03.004

Joback Method: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1484

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume