2-Amino-3-(4-hydroxyphenyl)-propanoic acid

Other names: DL-Tyrosine
(.+/-.)-Tyrosine
Tyrosine, DL-
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)
InchiKey: OUYCCCASQSFEME-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: NC(Cc1ccc(O)cc1)C(=O)O
Mol. weight [g/mol]: 181.19
CAS: 556-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-219.04	kJ/mol	Joback Method
hf	-406.17	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-0.89		Crippen Method
logp	0.347		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C556036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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