DL-3-hydroxyphenylalanine

Other names: 2-amino-3-(3-hydroxyphenyl)propanoic acid
DL-m-tyrosine
Inchi: InChI=1S/C9H11NO3/c10-8(9(12)13)5-6-2-1-3-7(11)4-6/h1-4,8,11H,5,10H2,(H,12,13)
InchiKey: JZKXXXDKRQWDET-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: NC(Cc1cccc(O)c1)C(=O)O
Mol. weight [g/mol]: 181.19

Physical Properties

Property code	Value	Unit	Source
hf	-456.16	kJ/mol	Cheméo Relay (1.0)
hfus	26.25	kJ/mol	Joback Method
hvap	110.79	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-0.63		Cheméo Relay (1.0)
logp	0.347		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
tb	592.93	K	Cheméo Relay (1.0)
tc	852.12	K	Cheméo Relay (1.0)
tf	478.30	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Binary Diffusion Coefficients of Aqueous Phenylalanine, Tyrosine Isomers, and Aminobutyric Acids at Infinitesimal Concentration and Temperatures from (293.2 to 333.2) K:	https://www.doi.org/10.1021/je3012698
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point