

Glycyl-L-tyrosine

Other names:	L-Tyrosine, N-glycyl-N-glycyl-L-tyrosine
Inchi:	InChI=1S/C11H14N2O4/c12-6-10(15)13-9(11(16)17)5-7-1-3-8(14)4-2-7/h1-4,9,14H,5-6,1
InchiKey:	XBGGUPMXALFZOT-SECBINFHSA-N
Formula:	C11H14N2O4
SMILES:	NCC(=O)NC(Cc1ccc(O)cc1)C(=O)O
Mol. weight [g/mol]:	238.24
CAS:	658-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-241.73	kJ/mol	Joback Method
hf	-506.56	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	102.23	kJ/mol	Joback Method
log10ws	-0.73		Aqueous Solubility Prediction Method
logp	-0.537		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	880.56	K	Joback Method
tc	1104.17	K	Joback Method
tf	633.47	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.10	J/molxK	880.56	Joback Method
cpg	542.17	J/molxK	917.83	Joback Method
cpg	550.82	J/molxK	955.10	Joback Method
cpg	559.16	J/molxK	992.37	Joback Method
cpg	567.26	J/molxK	1029.63	Joback Method
cpg	575.21	J/molxK	1066.90	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C658797&Units=SI>

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

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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

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