3,5-Diiodo-L-tyrosine

Other names:	2-amino-3-(4-hydroxy-3,5-diiodophenyl)propanoic acid
	3,5-Diiodotyrocine
	3,5-Iodo-L-tyrosine
	3,5-L-Diiodotyrosine
	DIT (amino acid)
	L-3,5-Diiodotyrosine
	L-Tyrosine, 3,5-diiodo-
	NSC 4143
	Tryosine, 3,5-diiodo-
	Tyrosine, 3,5-diiodo-, L-
Inchi:	InChI=1S/C9H9I2NO3/c10-5-1-4(2-6(11)8(5)13)3-7(12)9(14)15/h1-2,7,13H,3,12H2,(H,14
InchiKey:	NYPYHUZRZVSYKL-SSDOTTSWSA-N
Formula:	C9H9I2NO3
SMILES:	NC(Cc1cc(I)c(O)c(I)c1)C(=O)O
Mol. weight [g/mol]:	432.98
CAS:	300-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-122.06	kJ/mol	Joback Method
hf	-275.37	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	104.67	kJ/mol	Joback Method
log10ws	-2.86		Aqueous Solubility Prediction Method
logp	1.556		Crippen Method
mcvol	188.840	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	927.00	K	Joback Method
tc	1193.10	K	Joback Method
tf	649.50	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.45	J/mol×K	927.00	Joback Method
cpg	439.05	J/mol×K	971.35	Joback Method
cpg	446.74	J/mol×K	1015.70	Joback Method
cpg	454.67	J/mol×K	1060.05	Joback Method
cpg	463.00	J/mol×K	1104.40	Joback Method
cpg	471.87	J/mol×K	1148.75	Joback Method
cpg	481.44	J/mol×K	1193.10	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C300390&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