

N-methyl tyrosine

Other names:	Surinamine
Inchi:	InChI=1S/C10H13NO3/c1-11-9(10(13)14)6-7-2-4-8(12)5-3-7/h2-5,9,11-12H,6H2,1H3,(H,
InchiKey:	AXDLCFOOGCNDST-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	CNC(Cc1ccc(O)cc1)C(=O)O
Mol. weight [g/mol]:	195.22
CAS:	19897-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-187.68	kJ/mol	Joback Method
hf	-407.13	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.607		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	731.28	K	Joback Method
tc	944.40	K	Joback Method
tf	489.01	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.49	J/molxK	731.28	Joback Method
cpg	430.40	J/molxK	766.80	Joback Method
cpg	439.72	J/molxK	802.32	Joback Method
cpg	448.52	J/molxK	837.84	Joback Method
cpg	456.89	J/molxK	873.36	Joback Method
cpg	464.89	J/molxK	908.88	Joback Method
cpg	472.60	J/molxK	944.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19897633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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