Neostigmine

Other names:	Ammonium, (m-hydroxyphenyl)trimethyl-, dimethylcarbamate
	Benzenaminium, 3-(((dimethylamino)carbonyl)oxy)-N,N,N-trimethyl-
	Eustigmin
	Eustigmine
	(m-Hydroxyphenyl)trimethylammonium dimethylcarbamate
	Prostigmin
	Prostigmine
	Vagostigmine
	3-[[(Dimethylamino)carbonyl]oxy]-N,N,N-trimethylbenzenaminium
	Proserine
	Synstigmin
	Synstigmine
	(m-Hydroxyphenyl)dimethylamine dimethylcarbamate
Inchi:	InChI=1S/C12H19N2O2/c1-13(2)12(15)16-11-8-6-7-10(9-11)14(3,4)5/h6-9H,1-5H3/q+1
InchiKey:	ALWKGYPQUAPLQC-UHFFFAOYSA-N
Formula:	C12H19N2O2
SMILES:	CN(C)C(=O)Oc1cccc([N+](C)(C)C)c1
Mol. weight [g/mol]:	223.29
CAS:	59-99-4

Physical Properties

Property code	Value	Unit	Source
gf	88.20	kJ/mol	Joback Method
hf	-231.50	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	58.63	kJ/mol	Joback Method
log10ws	3.06		Crippen Method
logp	1.944		Crippen Method
mcvol	185.730	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
tb	607.49	K	Joback Method
tc	811.98	K	Joback Method
tf	384.67	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.73	J/mol×K	607.49	Joback Method
cpg	494.72	J/mol×K	641.57	Joback Method
cpg	510.74	J/mol×K	675.65	Joback Method
cpg	525.80	J/mol×K	709.73	Joback Method
cpg	539.92	J/mol×K	743.81	Joback Method
cpg	553.10	J/mol×K	777.90	Joback Method
cpg	565.35	J/mol×K	811.98	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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