(.+/-.)-Octopamine, N,N,O,O'-tetramethyl-

Inchi: InChI=1S/C12H19NO2/c1-13(2)9-12(15-4)10-5-7-11(14-3)8-6-10/h5-8,12H,9H2,1-4H3
InchiKey: JZJAYENCRJNUNQ-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: COc1ccc(C(CN(C)C)OC)cc1
Mol. weight [g/mol]: 209.28

Physical Properties

Property code	Value	Unit	Source
gf	51.28	kJ/mol	Joback Method
hf	-268.14	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.944		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	562.46	K	Joback Method
tc	761.09	K	Joback Method
tf	325.87	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.99	J/mol×K	562.46	Joback Method
cpg	451.70	J/mol×K	595.56	Joback Method
cpg	467.58	J/mol×K	628.67	Joback Method
cpg	482.63	J/mol×K	661.77	Joback Method
cpg	496.88	J/mol×K	694.88	Joback Method
cpg	510.33	J/mol×K	727.98	Joback Method
cpg	523.00	J/mol×K	761.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume