Dopamine, N,N-dimethyl-, dimethyl ether

Other names: 2-(3,4-Dimethoxyphenyl)-N,N-dimethylethanamine
Inchi: InChI=1S/C12H19NO2/c1-13(2)8-7-10-5-6-11(14-3)12(9-10)15-4/h5-6,9H,7-8H2,1-4H3
InchiKey: UNASPKKHQRCVGR-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: COc1ccc(CCN(C)C)cc1OC
Mol. weight [g/mol]: 209.28

Physical Properties

Property code	Value	Unit	Source
gf	44.09	kJ/mol	Joback Method
hf	-274.33	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.808		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1615.10		NIST Webbook
tb	567.88	K	Joback Method
tc	763.54	K	Joback Method
tf	353.39	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.81	J/mol×K	567.88	Joback Method
cpg	450.87	J/mol×K	600.49	Joback Method
cpg	466.18	J/mol×K	633.10	Joback Method
cpg	480.74	J/mol×K	665.71	Joback Method
cpg	494.57	J/mol×K	698.32	Joback Method
cpg	507.67	J/mol×K	730.93	Joback Method
cpg	520.05	J/mol×K	763.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332898&Units=SI

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