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]: 209.29

Physical Properties

Property code	Value	Unit	Source
hfus	25.50	kJ/mol	Joback Method
ie	7.80	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	1.808		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
rinpol	1615.10		NIST Webbook
tb	552.86	K	Cheméo Relay (1.0)
tf	337.63	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332898&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point