Tyramine, N,N-dimethyl-, methyl ether

Inchi: InChI=1S/C11H17NO/c1-12(2)9-8-10-4-6-11(13-3)7-5-10/h4-7H,8-9H2,1-3H3
InchiKey: BGSZBHCYLIHECZ-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: COc1ccc(CCN(C)C)cc1
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
gf	150.30	kJ/mol	Joback Method
hf	-110.00	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.799		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1430.30		NIST Webbook
rinpol	1430.30		NIST Webbook
tb	517.60	K	Joback Method
tc	716.53	K	Joback Method
tf	307.37	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.27	J/mol×K	517.60	Joback Method
cpg	376.25	J/mol×K	550.75	Joback Method
cpg	391.41	J/mol×K	583.91	Joback Method
cpg	405.79	J/mol×K	617.06	Joback Method
cpg	419.39	J/mol×K	650.22	Joback Method
cpg	432.25	J/mol×K	683.37	Joback Method
cpg	444.38	J/mol×K	716.53	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=U352573&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