3-Hydroxytyramine, N,O,O'-tris(trifluoroacetyl)-

Other names: Dopamine, TFA
Inchi: InChI=1S/C14H8F9NO5/c15-12(16,17)9(25)24-4-3-6-1-2-7(28-10(26)13(18,19)20)8(5-6)
InchiKey: ROWYZKLUWDEHTH-UHFFFAOYSA-N
Formula: C14H8F9NO5
SMILES: O=C(NCCc1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 441.20

Physical Properties

Property code	Value	Unit	Source
gf	-2091.99	kJ/mol	Joback Method
hf	-2458.65	kJ/mol	Joback Method
hfus	43.03	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	2.843		Crippen Method
mcvol	226.720	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1575.00		NIST Webbook
tb	796.72	K	Joback Method
tc	983.13	K	Joback Method
tf	558.48	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.34	J/mol×K	796.72	Joback Method
cpg	689.23	J/mol×K	827.79	Joback Method
cpg	697.35	J/mol×K	858.86	Joback Method
cpg	704.76	J/mol×K	889.93	Joback Method

cpg	711.50	J/mol×K	920.99	Joback Method
cpg	717.63	J/mol×K	952.06	Joback Method
cpg	723.19	J/mol×K	983.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375507&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

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