Tyramine, N-acetate, PFP

Inchi: InChI=1S/C13H12F5NO3/c1-8(20)19-7-6-9-2-4-10(5-3-9)22-11(21)12(14,15)13(16,17)18
InchiKey: RTGQZZWDYOIRTD-UHFFFAOYSA-N
Formula: C13H12F5NO3
SMILES: CC(=O)NCCc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 325.23

Physical Properties

Property code	Value	Unit	Source
gf	-1080.46	kJ/mol	Joback Method
hf	-1388.55	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.468		Crippen Method
mcvol	198.110	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	698.72	K	Joback Method
tc	889.95	K	Joback Method
tf	457.75	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.12	J/mol×K	698.72	Joback Method
cpg	570.76	J/mol×K	730.59	Joback Method
cpg	581.56	J/mol×K	762.46	Joback Method
cpg	591.55	J/mol×K	794.34	Joback Method
cpg	600.80	J/mol×K	826.21	Joback Method
cpg	609.34	J/mol×K	858.08	Joback Method
cpg	617.23	J/mol×K	889.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R539589&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