Octopamine, N-acetyl-TFA

Other names: p-Octopamine, N-acetate, TFA
Inchi: InChI=1S/C14H11F6NO5/c1-7(22)21-6-10(26-12(24)14(18,19)20)8-2-4-9(5-3-8)25-11(23
InchiKey: CIIQXYYPXUOIGW-UHFFFAOYSA-N
Formula: C14H11F6NO5
SMILES: CC(=O)NCC(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 387.23

Physical Properties

Property code	Value	Unit	Source
gf	-1503.21	kJ/mol	Joback Method
hf	-1855.38	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	73.31	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.437		Crippen Method
mcvol	221.410	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
tb	796.72	K	Joback Method
tc	991.35	K	Joback Method
tf	526.77	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.43	J/mol×K	796.72	Joback Method
cpg	667.40	J/mol×K	829.16	Joback Method
cpg	676.52	J/mol×K	861.60	Joback Method
cpg	684.83	J/mol×K	894.03	Joback Method
cpg	692.38	J/mol×K	926.47	Joback Method
cpg	699.20	J/mol×K	958.91	Joback Method
cpg	705.35	J/mol×K	991.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57238&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