m-Octopamine, TFA

Inchi: InChI=1S/C14H8F9NO5/c15-12(16,17)9(25)24-5-8(29-11(27)14(21,22)23)6-1-3-7(4-2-6)
InchiKey: AOQZMQBDUJCRTH-UHFFFAOYSA-N
Formula: C14H8F9NO5
SMILES: O=C(NCC(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 441.20

Physical Properties

Property code	Value	Unit	Source
gf	-2084.80	kJ/mol	Joback Method
hf	-2452.46	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.979		Crippen Method
mcvol	226.720	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	791.30	K	Joback Method
tc	978.20	K	Joback Method
tf	530.96	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.59	J/mol×K	791.30	Joback Method
cpg	691.62	J/mol×K	822.45	Joback Method
cpg	699.87	J/mol×K	853.60	Joback Method
cpg	707.37	J/mol×K	884.75	Joback Method
cpg	714.18	J/mol×K	915.90	Joback Method
cpg	720.36	J/mol×K	947.05	Joback Method
cpg	725.96	J/mol×K	978.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R529809&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