Octopamine, N-acetyl-PFP

Other names: p-Octopamine, N-acetate, PFP
Inchi: InChI=1S/C16H11F10NO5/c1-7(28)27-6-10(32-12(30)14(19,20)16(24,25)26)8-2-4-9(5-3-
InchiKey: WTUDMLSCVPBFBE-UHFFFAOYSA-N
Formula: C16H11F10NO5
SMILES: CC(=O)NCC(OC(=O)C(F)(F)C(F)(F)F)c1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 487.25

Physical Properties

Property code	Value	Unit	Source
gf	-2259.93	kJ/mol	Joback Method
hf	-2698.60	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.708		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook
tb	833.10	K	Joback Method
tc	1023.99	K	Joback Method
tf	556.51	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.71	J/mol×K	833.10	Joback Method
cpg	809.20	J/mol×K	864.92	Joback Method
cpg	817.88	J/mol×K	896.73	Joback Method
cpg	825.80	J/mol×K	928.55	Joback Method
cpg	833.06	J/mol×K	960.36	Joback Method
cpg	839.72	J/mol×K	992.18	Joback Method

cpg	845.87	J/mol×K	1023.99	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=R57224&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