Octopamine, tri-PFP

Other names: Octopamine, N,O,O-(tris-PFP)-
(.+/-.)-Octopamine, N,O,O'-tris(pentafluoropropionyl)-

Inchi: InChI=1S/C17H8F15NO5/c18-12(19,15(24,25)26)9(34)33-5-8(38-11(36)14(22,23)17(30,
4-(2-[(2,2,3,3,3-Pentafluoropropanoyl)amino]-1-[(2,2,3,3,3-pentafluoropropanoyl)oxy]ethy
2,2,3,3,3-pentafluoropropanoate

InchiKey: NAEIJMBSQQFJIL-UHFFFAOYSA-N

Formula: C17H8F15NO5

SMILES: O=C(NCC(OC(=O)C(F)(F)C(F)(F)F)c1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 591.23

CAS: 62237-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-3219.88	kJ/mol	Joback Method
hf	-3717.29	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	4.885		Crippen Method
mcvol	279.610	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	845.87	K	Joback Method
tc	1035.59	K	Joback Method
tf	575.57	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.03	J/mol×K	845.87	Joback Method
cpg	903.74	J/mol×K	877.49	Joback Method
cpg	911.68	J/mol×K	909.11	Joback Method
cpg	918.94	J/mol×K	940.73	Joback Method

cpg	925.66	J/mol×K	972.35	Joback Method
cpg	931.93	J/mol×K	1003.97	Joback Method
cpg	937.86	J/mol×K	1035.59	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=C62237949&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