

Dopamine, N-acetyl-PFP

Other names:	Dopamine, N-acetate, PFP
Inchi:	InChI=1S/C16H11F10NO5/c1-7(28)27-5-4-8-2-3-9(31-11(29)13(17,18)15(21,22)23)10(6-
InchiKey:	GVHOVUNEKLULSA-UHFFFAOYSA-N
Formula:	C16H11F10NO5
SMILES:	CC(=O)NCCc1ccc(OC(=O)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]:	487.25

Physical Properties

Property code	Value	Unit	Source
gf	-2267.12	kJ/mol	Joback Method
hf	-2704.79	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.571		Crippen Method
mcpvol	256.670	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	838.52	K	Joback Method
tc	1029.51	K	Joback Method
tf	584.03	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.53	J/molxK	838.52	Joback Method
cpg	806.92	J/molxK	870.35	Joback Method
cpg	815.52	J/molxK	902.18	Joback Method
cpg	823.39	J/molxK	934.02	Joback Method
cpg	830.60	J/molxK	965.85	Joback Method
cpg	837.24	J/molxK	997.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57206&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
mccvol:	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

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