

Propanoic acid, pentafluoro-, 4-[2-[(2,2,3,3,3-pentafluoro-1-oxopropyl)amino]ethylester

Other names:

N,O,O'-Tris(pentafluoropropionyl)dopamine

3-Hydroxytyramine, N,O,O'-tris(pentafluoropropionyl)-

Inchi: InChI=1S/C17H8F15NO5/c18-12(19,15(24,25)26)9(34)33-4-3-6-1-2-7(37-10(35)13(20,21

InchiKey: UHOMWVNKFQGMSSMM-UHFFFAOYSA-N

Formula: C17H8F15NO5

SMILES: O=C(NCCc1ccc(OC(=O)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 591.23

CAS: 59785-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-3227.07	kJ/mol	Joback Method
hf	-3723.48	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	4.749		Crippen Method
mcvol	279.610	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
tb	851.29	K	Joback Method
tc	1042.27	K	Joback Method
tf	603.09	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.74	J/molxK	851.29	Joback Method
cpg	901.41	J/molxK	883.12	Joback Method
cpg	909.32	J/molxK	914.95	Joback Method
cpg	916.59	J/molxK	946.78	Joback Method
cpg	923.31	J/molxK	978.61	Joback Method

cpg	929.61	J/mol×K	1010.44	Joback Method
cpg	935.58	J/mol×K	1042.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59785385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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