

Spermidine, N,N',N''-tris(pentafluoropropionyl)-

Other names:	2,2,3,3,3-Pentafluoro-N-(4-[(2,2,3,3,3-pentafluoropropanoyl)amino]butyl)-N-(3-[(2,2,3,3,3-pentafluoropropanoyl)amino]propyl)-N-(3-[(2,2,3,3,3-pentafluoropropanoyl)amino]propyl)butylamine
Inchi:	InChI=1S/C16H16F15N3O3/c17-11(18,14(23,24)25)8(35)32-4-1-2-6-34(10(37)13(21,22)14)16
InchiKey:	GFDNBHOLQEQME-UHFFFAOYSA-N
Formula:	C16H16F15N3O3
SMILES:	O=C(N(CCCCN=C(O)C(F)(F)C(F)(F)F)CCCN=C(O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	583.29
CAS:	71387-77-4

Physical Properties

Property code	Value	Unit	Source
hf	-3572.37	kJ/mol	Joback Method
hvap	80.11	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.491		Crippen Method
mcvol	297.500	ml/mol	McGowan Method
pc	935.20	kPa	Joback Method
rinpol	1868.20		NIST Webbook
rinpol	1868.20		NIST Webbook
tb	938.94	K	Joback Method
tc	1175.36	K	Joback Method

Sources

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=C71387774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinqol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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