

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

Inchi: InChI=1S/C13H16F9N3O3/c14-11(15,16)8(26)23-4-1-2-6-25(10(28)13(20,21)22)7-3-5-24
InchiKey: JSBLZFOYYFWYPH-UHFFFAOYSA-N
Formula: C13H16F9N3O3
SMILES: O=C(N(CCCCN=C(O)C(F)(F)F)CCCN=C(O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 433.27

Physical Properties

Property code	Value	Unit	Source
hf	-2307.54	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.585		Crippen Method
mcvol	244.610	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	1946.70		NIST Webbook
rinpol	1946.70		NIST Webbook
tb	884.37	K	Joback Method
tc	1085.69	K	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=U352602&Units=SI>

Legend

hf: Enthalpy of formation 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

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