N-(4-Aminobutyl)acetamide, N,N'-bis(trifluoroacetyl)

Other names: N-Acetyl-2,2,2-trifluoro-N-[4-(2,2,2-trifluoroacetamido)butyl]acetamide
Inchi: InChI=1S/C10H12F6N2O3/c1-6(19)18(8(21)10(14,15)16)5-3-2-4-17-7(20)9(11,12)13/h2-
InchiKey: VENILQKZFRWLKU-UHFFFAOYSA-N
Formula: C10H12F6N2O3
SMILES: CC(=O)N(CCCCN=C(O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 322.20

Physical Properties

Property code	Value	Unit	Source
hf	-1681.32	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.223		Crippen Method
mcvol	187.050	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1442.00		NIST Webbook
tb	706.28	K	Joback Method
tc	877.35	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=U378747&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