5-amino-1-pentanol, N,O-bis(trifluoroacetyl)-

Inchi: InChI=1S/C9H11F6NO3/c10-8(11,12)6(17)16-4-2-1-3-5-19-7(18)9(13,14)15/h1-5H2,(H,1
InchiKey: UWXZRWAWQZRDIT-UHFFFAOYSA-N
Formula: C9H11F6NO3
SMILES: O=C(NCCCCCOC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 295.18

Physical Properties

Property code	Value	Unit	Source
gf	-1411.73	kJ/mol	Joback Method
hf	-1727.16	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	50.47	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.941		Crippen Method
mcvol	167.280	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1265.00		NIST Webbook
rinpol	1265.00		NIST Webbook
tb	574.81	K	Joback Method
tc	734.75	K	Joback Method
tf	374.32	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.65	J/mol×K	574.81	Joback Method
cpg	459.49	J/mol×K	601.47	Joback Method
cpg	469.73	J/mol×K	628.12	Joback Method
cpg	479.38	J/mol×K	654.78	Joback Method
cpg	488.47	J/mol×K	681.44	Joback Method
cpg	497.02	J/mol×K	708.09	Joback Method
cpg	505.07	J/mol×K	734.75	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=U374916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume