2-(isopropyl(trifluoroacetyl)amino)ethyl trifluoroacetate

Other names: 2-(N-Isopropyl-trifluoroacetylamino)ethanol trifluoroacetate
(N-Trifluoroacetyloxyethyl)isopropyl-trifluoroacetylamine

Inchi: InChI=1S/C9H11F6NO3/c1-5(2)16(6(17)8(10,11)12)3-4-19-7(18)9(13,14)15/h5H,3-4H2,1

InchiKey: KTOOQRYBIWTNRO-UHFFFAOYSA-N

Formula: C9H11F6NO3

SMILES: CC(C)N(CCOC(=O)C(F)(F)F)C(=O)C(F)(F)F

Mol. weight [g/mol]: 295.18

Physical Properties

Property code	Value	Unit	Source
gf	-1392.78	kJ/mol	Joback Method
hf	-1718.38	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	45.69	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.891		Crippen Method
mcvol	167.280	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1067.00		NIST Webbook
tb	536.64	K	Joback Method
tc	694.65	K	Joback Method
tf	339.13	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.37	J/mol×K	536.64	Joback Method
cpg	446.09	J/mol×K	562.97	Joback Method
cpg	457.14	J/mol×K	589.31	Joback Method
cpg	467.56	J/mol×K	615.64	Joback Method
cpg	477.38	J/mol×K	641.98	Joback Method
cpg	486.61	J/mol×K	668.31	Joback Method
cpg	495.29	J/mol×K	694.65	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=U373297&Units=SI

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