BENZENETHANAMINE, N-TFA-3,4-DIMETHOXY-

Other names: Benzenethanamine, N-trifluoroacetyl-3,4-dimethoxy-
Benzenethanamine, N-TFA-4,5-dimethoxy-
Benzeneethanamine, 3,4-dimethoxy-N-TFA-

Inchi: InChI=1S/C12H14F3NO3/c1-18-9-4-3-8(7-10(9)19-2)5-6-16-11(17)12(13,14)15/h3-4,7H,

InchiKey: RIULCRYOMGKNSV-UHFFFAOYSA-N

Formula: C12H14F3NO3

SMILES: COc1ccc(CCNC(=O)C(F)(F)F)cc1OC

Mol. weight [g/mol]: 277.24

Physical Properties

Property code	Value	Unit	Source
hfus	31.00	kJ/mol	Joback Method
ie	8.67	eV	Cheméo Relay (1.0)
logp	1.925		Crippen Method
mcvol	184.780	ml/mol	McGowan Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	570.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.76	J/mol×K	654.06	Joback Method
cpg	510.63	J/mol×K	685.97	Joback Method
cpg	522.75	J/mol×K	717.87	Joback Method
cpg	534.12	J/mol×K	749.78	Joback Method
cpg	544.76	J/mol×K	781.68	Joback Method
cpg	554.69	J/mol×K	813.59	Joback Method
cpg	563.93	J/mol×K	845.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13230712&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature