

3,4-Dimethoxyphenylethylamine, N-trifluoroacetyl-

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
CAS:	13230-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-687.81	kJ/mol	Joback Method
hf	-998.05	kJ/mol	Joback Method
hfus	31.00	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.925		Crippen Method
mcvol	184.780	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	654.06	K	Joback Method
tc	845.49	K	Joback Method
tf	427.70	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.76	J/molxK	654.06	Joback Method
cpg	510.63	J/molxK	685.97	Joback Method
cpg	522.75	J/molxK	717.87	Joback Method
cpg	534.12	J/molxK	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13230712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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

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