

2-(2,5-Dimethoxy-4-ethylphenyl)ethylamine, N-trifluoroacetyl-

Other names:	4-ethyl-2,5-dimethoxy-«beta»-phenethylamine, TFA
Inchi:	InChI=1S/C14H18F3NO3/c1-4-9-7-12(21-3)10(8-11(9)20-2)5-6-18-13(19)14(15,16)17/h7
InchiKey:	BORZZNXPOVRTQG-UHFFFAOYSA-N
Formula:	C14H18F3NO3
SMILES:	CCc1cc(OC)c(CCNC(=O)C(F)(F)F)cc1OC
Mol. weight [g/mol]:	305.29

Physical Properties

Property code	Value	Unit	Source
gf	-680.60	kJ/mol	Joback Method
hf	-1050.80	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.487		Crippen Method
mcvol	212.960	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	704.80	K	Joback Method
tc	894.06	K	Joback Method
tf	462.76	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.22	J/molxK	704.80	Joback Method
cpg	614.93	J/molxK	736.34	Joback Method
cpg	627.83	J/molxK	767.89	Joback Method
cpg	639.94	J/molxK	799.43	Joback Method
cpg	651.28	J/molxK	830.97	Joback Method
cpg	661.86	J/molxK	862.52	Joback Method
cpg	671.70	J/molxK	894.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360351&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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