2,5-Dimethoxy-4-methyl-«beta»-phenethylamine, TFA

InChI: InChI=1S/C13H16F3NO3/c1-8-6-11(20-3)9(7-10(8)19-2)4-5-17-12(18)13(14,15)16/h6-7H
InchiKey: VRWAKTQPXNNYMC-UHFFFAOYSA-N
Formula: C13H16F3NO3
SMILES: COc1cc(CCNC(=O)C(F)(F)F)c(OC)cc1C
Mol. weight [g/mol]: 291.27

Physical Properties

Property code	Value	Unit	Source
gf	-689.02	kJ/mol	Joback Method
hf	-1030.16	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	63.05	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.233		Crippen Method
mcvol	198.870	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	681.92	K	Joback Method
tc	872.49	K	Joback Method
tf	451.49	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.41	J/mol×K	681.92	Joback Method
cpg	561.65	J/mol×K	713.68	Joback Method
cpg	574.12	J/mol×K	745.44	Joback Method
cpg	585.84	J/mol×K	777.21	Joback Method
cpg	596.81	J/mol×K	808.97	Joback Method
cpg	607.05	J/mol×K	840.73	Joback Method
cpg	616.58	J/mol×K	872.49	Joback Method

Sources

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=R438387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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