4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-), isomer 2, di-TFA

Inchi: InChI=1S/C13H10F6INO4/c1-24-8-5-7(20)9(25-11(23)13(17,18)19)4-6(8)2-3-21-10(22)12
InchiKey: WFSYYMNUKYCWIJ-UHFFFAOYSA-N
Formula: C13H10F6INO4
SMILES: COc1cc(I)c(OC(=O)C(F)(F)F)cc1CCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 485.12

Physical Properties

Property code	Value	Unit	Source
gf	-1341.41	kJ/mol	Joback Method
hf	-1662.95	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	2.988		Crippen Method
mcvol	231.570	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	823.51	K	Joback Method
tc	1029.88	K	Joback Method
tf	563.67	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.59	J/mol×K	823.51	Joback Method
cpg	639.53	J/mol×K	857.90	Joback Method
cpg	647.70	J/mol×K	892.30	Joback Method
cpg	655.15	J/mol×K	926.69	Joback Method
cpg	661.92	J/mol×K	961.09	Joback Method
cpg	668.06	J/mol×K	995.48	Joback Method
cpg	673.62	J/mol×K	1029.88	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=R514644&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

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