Phenethylamine, 2,5-dimethoxy-4-propylthio, N-trifluoroacetyl

Inchi: InChI=1S/C15H20F3NO3S/c1-4-7-23-13-9-11(21-2)10(8-12(13)22-3)5-6-19-14(20)15(16

InchiKey: GEOKSLHKIXGKIF-UHFFFAOYSA-N

Formula: C15H20F3NO3S

SMILES: CCCSc1cc(OC)c(CCNC(=O)C(F)(F)F)cc1OC

Mol. weight [g/mol]: 351.38

Physical Properties

Property code	Value	Unit	Source
gf	-639.06	kJ/mol	Joback Method
hf	-1029.57	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.427		Crippen Method
mcvol	243.400	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2170.00		NIST Webbook
tb	796.46	K	Joback Method
tc	998.37	K	Joback Method
tf	508.43	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.78	J/mol×K	796.46	Joback Method
cpg	725.11	J/mol×K	830.11	Joback Method
cpg	737.45	J/mol×K	863.76	Joback Method
cpg	748.83	J/mol×K	897.41	Joback Method
cpg	759.26	J/mol×K	931.07	Joback Method
cpg	768.76	J/mol×K	964.72	Joback Method
cpg	777.33	J/mol×K	998.37	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=R418645&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