3,4-Dimethoxyphenylethylamine, N-pentafluoropropionyl-

Inchi: InChI=1S/C13H14F5NO3/c1-21-9-4-3-8(7-10(9)22-2)5-6-19-11(20)12(14,15)13(16,17)18

InchiKey: HMEFYKFJKZBVEA-UHFFFAOYSA-N

Formula: C13H14F5NO3

SMILES: COc1ccc(CCNC(=O)C(F)(F)C(F)(F)F)cc1OC

Mol. weight [g/mol]: 327.25

Physical Properties

Property code	Value	Unit	Source
gf	-1066.17	kJ/mol	Joback Method
hf	-1419.66	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	59.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.560		Crippen Method
mcvol	202.410	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	672.25	K	Joback Method
tc	856.63	K	Joback Method
tf	442.57	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.11	J/mol×K	672.25	Joback Method
cpg	580.81	J/mol×K	702.98	Joback Method
cpg	592.70	J/mol×K	733.71	Joback Method
cpg	603.81	J/mol×K	764.44	Joback Method
cpg	614.18	J/mol×K	795.17	Joback Method
cpg	623.84	J/mol×K	825.90	Joback Method
cpg	632.81	J/mol×K	856.63	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=U374332&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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