Benzenethanamine, 3,4,5-trimethoxy-«alpha»-methyl-(.+/-.)-

Inchi: InChI=1S/C12H19NO3/c1-8(13)5-9-6-10(14-2)12(16-4)11(7-9)15-3/h6-8H,5,13H2,1-4H3
InchiKey: WGTASENVNYJZBK-UHFFFAOYSA-N
Formula: C12H19NO3
SMILES: COc1cc(CC(C)N)cc(OC)c1OC
Mol. weight [g/mol]: 225.28
CAS: 22199-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-117.31	kJ/mol	Joback Method
hf	-457.04	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
ie	8.16 ± 0.06	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	1.602		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	654.93	K	Joback Method
tc	864.02	K	Joback Method
tf	423.93	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.94	J/mol×K	654.93	Joback Method
cpg	504.12	J/mol×K	689.78	Joback Method
cpg	518.51	J/mol×K	724.63	Joback Method
cpg	532.11	J/mol×K	759.48	Joback Method
cpg	544.90	J/mol×K	794.33	Joback Method
cpg	556.85	J/mol×K	829.17	Joback Method
cpg	567.95	J/mol×K	864.02	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=C22199173&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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