Benzeneethanamine,2,5-dimethoxy-«alpha»-meth

Inchi: InChI=1S/C12H19NO2S/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-8H,5,13H2,1-4H
InchiKey: COBYBOVXXDQRAU-UHFFFAOYSA-N
Formula: C12H19NO2S
SMILES: COc1cc(SC)c(OC)cc1CC(C)N
Mol. weight [g/mol]: 241.35
CAS: 69519-59-1

Physical Properties

Property code	Value	Unit	Source
gf	20.81	kJ/mol	Joback Method
hf	-282.95	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
ie	7.64 ± 0.06	eV	NIST Webbook
log10ws	-3.22		Crippen Method
logp	2.315		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	701.29	K	Joback Method
tc	928.12	K	Joback Method
tf	436.10	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.01	J/mol×K	701.29	Joback Method
cpg	533.23	J/mol×K	739.10	Joback Method
cpg	547.47	J/mol×K	776.90	Joback Method
cpg	560.73	J/mol×K	814.71	Joback Method
cpg	572.97	J/mol×K	852.51	Joback Method
cpg	584.20	J/mol×K	890.32	Joback Method
cpg	594.39	J/mol×K	928.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69519591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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