Methoxyphenamine acetate

Other names: R,S-N-methyl-1-(2-methoxyphenyl)-2-aminopropane, AC
Inchi: InChI=1S/C13H19NO2/c1-10(14(3)11(2)15)9-12-7-5-6-8-13(12)16-4/h5-8,10H,9H2,1-4H3
InchiKey: VHZBAKZCZIEIJH-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: COc1ccccc1CC(C)N(C)C(C)=O
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	35.78	kJ/mol	Joback Method
hf	-269.14	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	58.28	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.104		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	616.79	K	Joback Method
tc	821.95	K	Joback Method
tf	364.84	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.95	J/mol×K	616.79	Joback Method
cpg	497.26	J/mol×K	650.98	Joback Method
cpg	512.63	J/mol×K	685.18	Joback Method
cpg	527.07	J/mol×K	719.37	Joback Method
cpg	540.63	J/mol×K	753.56	Joback Method
cpg	553.32	J/mol×K	787.76	Joback Method
cpg	565.18	J/mol×K	821.95	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=U123255&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