4-Ethoxy-3-methoxyphenethylamine

Inchi: InChI=1S/C11H17NO2/c1-3-14-10-5-4-9(6-7-12)8-11(10)13-2/h4-5,8H,3,6-7,12H2,1-2H3
InchiKey: AFMUTJRFLRYILG-UHFFFAOYSA-N
Formula: C11H17NO2
SMILES: CCOc1ccc(CCN)cc1OC
Mol. weight [g/mol]: 195.26
CAS: 36377-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-8.66	kJ/mol	Joback Method
hf	-287.43	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.595		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	605.09	K	Joback Method
tc	814.70	K	Joback Method
tf	392.91	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.91	J/mol×K	605.09	Joback Method
cpg	427.50	J/mol×K	640.03	Joback Method
cpg	441.37	J/mol×K	674.96	Joback Method
cpg	454.50	J/mol×K	709.90	Joback Method
cpg	466.90	J/mol×K	744.83	Joback Method
cpg	478.57	J/mol×K	779.77	Joback Method
cpg	489.50	J/mol×K	814.70	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=C36377590&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume