4-Phenoxyphenethylamine

Inchi: InChI=1S/C14H15NO/c15-11-10-12-6-8-14(9-7-12)16-13-4-2-1-3-5-13/h1-9H,10-11,15H2
InchiKey: JNHPLGDXCJAUBX-UHFFFAOYSA-N
Formula: C14H15NO
SMILES: NCCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 213.28
CAS: 118468-18-1

Physical Properties

Property code	Value	Unit	Source
gf	243.64	kJ/mol	Joback Method
hf	30.87	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.980		Crippen Method
mcvol	176.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	673.01	K	Joback Method
tc	916.29	K	Joback Method
tf	418.39	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.70	J/mol×K	673.01	Joback Method
cpg	475.55	J/mol×K	713.56	Joback Method
cpg	490.18	J/mol×K	754.10	Joback Method
cpg	503.65	J/mol×K	794.65	Joback Method
cpg	516.01	J/mol×K	835.20	Joback Method
cpg	527.32	J/mol×K	875.74	Joback Method
cpg	537.63	J/mol×K	916.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118468181&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
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