4-Phenoxybenzonitrile

Inchi: InChI=1S/C13H9NO/c14-10-11-6-8-13(9-7-11)15-12-4-2-1-3-5-12/h1-9H
InchiKey: UYHCIOZMFCLUDP-UHFFFAOYSA-N
Formula: C13H9NO
SMILES: N#Cc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 195.22
CAS: 3096-81-9

Physical Properties

Property code	Value	Unit	Source
gf	301.95	kJ/mol	Joback Method
hf	182.60	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.351		Crippen Method
mcvol	153.760	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	679.68	K	Joback Method
tc	934.70	K	Joback Method
tf	388.85	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.19	J/mol×K	679.68	Joback Method
cpg	385.96	J/mol×K	722.18	Joback Method
cpg	397.65	J/mol×K	764.69	Joback Method
cpg	408.30	J/mol×K	807.19	Joback Method
cpg	417.95	J/mol×K	849.69	Joback Method
cpg	426.67	J/mol×K	892.19	Joback Method
cpg	434.49	J/mol×K	934.70	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=C3096819&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