

4-Phenoxyphenylacetonitrile

Inchi:	InChI=1S/C14H11NO/c15-11-10-12-6-8-14(9-7-12)16-13-4-2-1-3-5-13/h1-9H,10H2
InchiKey:	PCOVIPKFOQOPEH-UHFFFAOYSA-N
Formula:	C14H11NO
SMILES:	N#CCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	209.24
CAS:	92163-15-0

Physical Properties

Property code	Value	Unit	Source
gf	310.37	kJ/mol	Joback Method
hf	161.96	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	64.86	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.545		Crippen Method
mcvol	167.850	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	702.56	K	Joback Method
tc	951.82	K	Joback Method
tf	400.12	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.31	J/molxK	702.56	Joback Method
cpg	436.69	J/molxK	744.10	Joback Method
cpg	448.95	J/molxK	785.65	Joback Method
cpg	460.15	J/molxK	827.19	Joback Method
cpg	470.34	J/molxK	868.73	Joback Method
cpg	479.57	J/molxK	910.27	Joback Method
cpg	487.90	J/molxK	951.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92163150&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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