2-Phenoxyphenylacetonitrile

Inchi: InChI=1S/C14H11NO/c15-11-10-12-6-4-5-9-14(12)16-13-7-2-1-3-8-13/h1-9H,10H2
InchiKey: PCMQCXFXODBYGN-UHFFFAOYSA-N
Formula: C14H11NO
SMILES: N#CCc1ccccc1Oc1ccccc1
Mol. weight [g/mol]: 209.24
CAS: 25562-98-5

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/mol×K	702.56	Joback Method
cpg	436.69	J/mol×K	744.10	Joback Method
cpg	448.95	J/mol×K	785.65	Joback Method
cpg	460.15	J/mol×K	827.19	Joback Method
cpg	470.34	J/mol×K	868.73	Joback Method
cpg	479.57	J/mol×K	910.27	Joback Method
cpg	487.90	J/mol×K	951.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25562985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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