3-PHENOXYPHENYLACETONITRILE

Other names: Benzeneacetonitrile, 3-phenoxy-
3-Phenoxybenzeneacetonitrile
m-Phenoxybenzyl cyanide
3-Phenoxybenzyl cyanide
(m-Phenoxyphenyl)acetonitrile
(3-Phenoxyphenyl)acetonitrile

Inchi: InChI=1S/C14H11NO/c15-10-9-12-5-4-8-14(11-12)16-13-6-2-1-3-7-13/h1-8,11H,9H2

InchiKey: DKGMALJGFUHPGB-UHFFFAOYSA-N

Formula: C14H11NO

SMILES: N#CCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 209.25

Physical Properties

Property code	Value	Unit	Source
af	0.5973		Cheméo Relay (1.0)
hf	169.80	kJ/mol	Cheméo Relay (1.0)
hfus	22.40	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-4.42		Cheméo Relay (1.0)
logp	3.545		Crippen Method
mcvol	167.850	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	621.60	K	Cheméo Relay (1.0)
tc	885.24	K	Cheméo Relay (1.0)
tf	319.97	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51632292&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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