Benzonitrile, 2-chloro-6-(phenylmethoxy)-

Other names:	2-Chloro-6-benzyloxybenzonitrile
	Benzonitrile, 2-benzyloxy-6-chloro-
Inchi:	InChI=1S/C14H10ClNO/c15-13-7-4-8-14(12(13)9-16)17-10-11-5-2-1-3-6-11/h1-8H,10H2
InchiKey:	CEFUICQUABSEPM-UHFFFAOYSA-N
Formula:	C14H10ClNO
SMILES:	N#Cc1c(Cl)cccc1OCc1ccccc1
Mol. weight [g/mol]:	243.69
CAS:	92161-40-5

Physical Properties

Property code	Value	Unit	Source
gf	288.81	kJ/mol	Joback Method
hf	134.75	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.791		Crippen Method
mcvol	180.090	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
tb	744.97	K	Joback Method
tc	997.06	K	Joback Method
tf	442.56	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.19	J/mol×K	744.97	Joback Method
cpg	456.18	J/mol×K	786.99	Joback Method
cpg	467.11	J/mol×K	829.00	Joback Method
cpg	477.03	J/mol×K	871.02	Joback Method
cpg	486.00	J/mol×K	913.03	Joback Method
cpg	494.06	J/mol×K	955.05	Joback Method
cpg	501.25	J/mol×K	997.06	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92161405&Units=SI

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