2-Chloro-6-benzyloxybenzonitrile

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

Physical Properties

Property code	Value	Unit	Source
hfus	26.21	kJ/mol	Joback Method
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-4.90		Cheméo Relay (1.0)
logp	3.791		Crippen Method
mcvol	180.090	ml/mol	McGowan Method
tb	627.78	K	Cheméo Relay (1.0)
tf	371.88	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92161405&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point