3-Chlorophenoxyacetonitrile

Inchi: InChI=1S/C8H6ClNO/c9-7-2-1-3-8(6-7)11-5-4-10/h1-3,6H,5H2
InchiKey: NHHNUPMHGVIQQC-UHFFFAOYSA-N
Formula: C8H6ClNO
SMILES: N#CCOc1cccc(Cl)c1
Mol. weight [g/mol]: 167.59
CAS: 43111-32-6

Physical Properties

Property code	Value	Unit	Source
gf	135.51	kJ/mol	Joback Method
hf	33.53	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.242		Crippen Method
mcvol	119.310	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	576.03	K	Joback Method
tc	810.18	K	Joback Method
tf	336.00	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.55	J/mol×K	576.03	Joback Method
cpg	252.76	J/mol×K	615.06	Joback Method
cpg	261.37	J/mol×K	654.08	Joback Method
cpg	269.41	J/mol×K	693.11	Joback Method
cpg	276.88	J/mol×K	732.13	Joback Method
cpg	283.79	J/mol×K	771.16	Joback Method
cpg	290.16	J/mol×K	810.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43111326&Units=SI
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

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