6-Chlorohexanoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C13H14ClNO2/c14-9-3-1-2-4-13(16)17-12-7-5-11(10-15)6-8-12/h5-8H,1-4,9H2
InchiKey: SDRUVBBNRXNYRO-UHFFFAOYSA-N
Formula: C13H14ClNO2
SMILES: N#Cc1ccc(OC(=O)CCCCCCl)cc1
Mol. weight [g/mol]: 251.71

Physical Properties

Property code	Value	Unit	Source
gf	48.69	kJ/mol	Joback Method
hf	-182.25	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.263		Crippen Method
mcvol	191.330	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	744.30	K	Joback Method
tc	964.13	K	Joback Method
tf	442.28	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.09	J/mol×K	744.30	Joback Method
cpg	506.88	J/mol×K	780.94	Joback Method
cpg	517.84	J/mol×K	817.58	Joback Method
cpg	527.97	J/mol×K	854.22	Joback Method
cpg	537.32	J/mol×K	890.85	Joback Method
cpg	545.90	J/mol×K	927.49	Joback Method
cpg	553.74	J/mol×K	964.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307623&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume