6-Chlorohexanoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C12H14ClNO4/c13-9-3-1-2-4-12(15)18-11-7-5-10(6-8-11)14(16)17/h5-8H,1-4,9
InchiKey: ILPNRCAJUCEDJY-UHFFFAOYSA-N
Formula: C12H14ClNO4
SMILES: O=C(CCCCCCl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 271.70

Physical Properties

Property code	Value	Unit	Source
gf	-57.36	kJ/mol	Joback Method
hf	-337.25	kJ/mol	Joback Method
hfus	38.83	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.299		Crippen Method
mcvol	193.280	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	771.18	K	Joback Method
tc	1002.24	K	Joback Method
tf	509.63	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.67	J/mol×K	771.18	Joback Method
cpg	532.75	J/mol×K	809.69	Joback Method
cpg	543.86	J/mol×K	848.20	Joback Method
cpg	554.04	J/mol×K	886.71	Joback Method
cpg	563.31	J/mol×K	925.22	Joback Method
cpg	571.72	J/mol×K	963.73	Joback Method
cpg	579.29	J/mol×K	1002.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307625&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

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