5-Chlorovaleric acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H12ClNO4/c12-8-2-1-3-11(14)17-10-6-4-9(5-7-10)13(15)16/h4-7H,1-3,8H2
InchiKey: XBBBWKBYQVWSPV-UHFFFAOYSA-N
Formula: C11H12ClNO4
SMILES: O=C(CCCCCl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 257.67

Physical Properties

Property code	Value	Unit	Source
gf	-65.78	kJ/mol	Joback Method
hf	-316.61	kJ/mol	Joback Method
hfus	36.24	kJ/mol	Joback Method
hvap	73.15	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.909		Crippen Method
mcvol	179.190	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	2043.00		NIST Webbook
tb	748.30	K	Joback Method
tc	983.47	K	Joback Method
tf	498.36	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.32	J/mol×K	748.30	Joback Method
cpg	479.93	J/mol×K	787.50	Joback Method
cpg	490.60	J/mol×K	826.69	Joback Method
cpg	500.36	J/mol×K	865.89	Joback Method
cpg	509.24	J/mol×K	905.08	Joback Method
cpg	517.27	J/mol×K	944.28	Joback Method
cpg	524.48	J/mol×K	983.47	Joback Method

Sources

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=U307980&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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