6-Chlorohexanoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C12H10ClF5O2/c13-5-3-1-2-4-6(19)20-12-10(17)8(15)7(14)9(16)11(12)18/h1-5

InchiKey: LUMHPBZXFFOIBC-UHFFFAOYSA-N

Formula: C12H10ClF5O2

SMILES: O=C(CCCCCCl)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 316.65

Physical Properties

Property code	Value	Unit	Source
gf	-1105.48	kJ/mol	Joback Method
hf	-1352.92	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	57.35	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.087		Crippen Method
mcvol	184.710	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1601.00		NIST Webbook
tb	635.61	K	Joback Method
tc	810.83	K	Joback Method
tf	419.05	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.61	J/mol×K	635.61	Joback Method
cpg	469.18	J/mol×K	664.81	Joback Method
cpg	479.27	J/mol×K	694.02	Joback Method
cpg	488.87	J/mol×K	723.22	Joback Method
cpg	497.99	J/mol×K	752.42	Joback Method
cpg	506.62	J/mol×K	781.63	Joback Method
cpg	514.76	J/mol×K	810.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354727&Units=SI

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