6-Chlorohexanoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C11H13ClF8O2/c12-5-3-1-2-4-7(21)22-6-9(15,16)11(19,20)10(17,18)8(13)14/h

InchiKey: HAVKFWBJGWWDNB-UHFFFAOYSA-N

Formula: C11H13ClF8O2

SMILES: O=C(CCCCCCl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 364.66

Physical Properties

Property code	Value	Unit	Source
gf	-1756.51	kJ/mol	Joback Method
hf	-2131.32	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	42.81	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.500		Crippen Method
mcvol	199.690	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
tb	548.83	K	Joback Method
tc	699.20	K	Joback Method
tf	312.79	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.55	J/mol×K	548.83	Joback Method
cpg	534.02	J/mol×K	573.89	Joback Method
cpg	545.78	J/mol×K	598.95	Joback Method
cpg	556.88	J/mol×K	624.01	Joback Method
cpg	567.34	J/mol×K	649.07	Joback Method
cpg	577.20	J/mol×K	674.14	Joback Method
cpg	586.48	J/mol×K	699.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354724&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