4-Chlorobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H7ClF8O2/c13-7-3-1-6(2-4-7)8(22)23-5-10(16,17)12(20,21)11(18,19)9(14)
InchiKey: IJXZGAWCZPWOKT-UHFFFAOYSA-N
Formula: C12H7ClF8O2
SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccc(Cl)cc1
Mol. weight [g/mol]: 370.62

Physical Properties

Property code	Value	Unit	Source
gf	-1645.31	kJ/mol	Joback Method
hf	-1926.90	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.668		Crippen Method
mcvol	190.020	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	603.37	K	Joback Method
tc	781.54	K	Joback Method
tf	363.00	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.07	J/mol×K	603.37	Joback Method
cpg	508.47	J/mol×K	633.06	Joback Method
cpg	519.00	J/mol×K	662.76	Joback Method
cpg	528.72	J/mol×K	692.45	Joback Method
cpg	537.67	J/mol×K	722.15	Joback Method
cpg	545.91	J/mol×K	751.84	Joback Method
cpg	553.49	J/mol×K	781.54	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=U354624&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