3-Chlorobenzoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C11H6ClF7O2/c12-7-3-1-2-6(4-7)8(20)21-5-9(13,14)10(15,16)11(17,18)19/h1-

InchiKey: YBUZSRFMUARWRZ-UHFFFAOYSA-N

Formula: C11H6ClF7O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)F)c1cccc(Cl)c1

Mol. weight [g/mol]: 338.61

Physical Properties

Property code	Value	Unit	Source
gf	-1456.48	kJ/mol	Joback Method
hf	-1704.87	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	46.95	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.330		Crippen Method
mcvol	174.160	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
tb	581.66	K	Joback Method
tc	765.71	K	Joback Method
tf	366.14	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.80	J/mol×K	581.66	Joback Method
cpg	451.94	J/mol×K	612.33	Joback Method
cpg	462.20	J/mol×K	643.01	Joback Method
cpg	471.63	J/mol×K	673.68	Joback Method
cpg	480.29	J/mol×K	704.36	Joback Method
cpg	488.22	J/mol×K	735.03	Joback Method
cpg	495.49	J/mol×K	765.71	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=U357391&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