3-Chlorobenzoic acid, pentafluorobenzyl ester

Inchi: InChI=1S/C14H6ClF5O2/c15-7-3-1-2-6(4-7)14(21)22-5-8-9(16)11(18)13(20)12(19)10(8)1
InchiKey: OAAVKYAFTYDFGI-UHFFFAOYSA-N
Formula: C14H6ClF5O2
SMILES: O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1cccc(Cl)c1
Mol. weight [g/mol]: 336.64

Physical Properties

Property code	Value	Unit	Source
gf	-985.86	kJ/mol	Joback Method
hf	-1169.14	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.393		Crippen Method
mcvol	189.130	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1850.00		NIST Webbook
tb	713.03	K	Joback Method
tc	915.85	K	Joback Method
tf	480.53	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.70	J/mol×K	713.03	Joback Method
cpg	482.86	J/mol×K	746.83	Joback Method
cpg	492.33	J/mol×K	780.64	Joback Method
cpg	501.12	J/mol×K	814.44	Joback Method
cpg	509.23	J/mol×K	848.24	Joback Method
cpg	516.66	J/mol×K	882.04	Joback Method
cpg	523.44	J/mol×K	915.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357396&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