2-Chloro-4-methoxyphenol, heptafluorobutyrate

Inchi: InChI=1S/C11H6ClF7O3/c1-21-5-2-3-7(6(12)4-5)22-8(20)9(13,14)10(15,16)11(17,18)19/

InchiKey: ICQDSAFHGWEURK-UHFFFAOYSA-N

Formula: C11H6ClF7O3

SMILES: COc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(Cl)c1

Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-1571.11	kJ/mol	Joback Method
hf	-1848.56	kJ/mol	Joback Method
hfus	25.00	kJ/mol	Joback Method
hvap	50.02	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.087		Crippen Method
mcvol	180.030	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
tb	609.06	K	Joback Method
tc	793.08	K	Joback Method
tf	400.89	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.91	J/mol×K	609.06	Joback Method
cpg	474.46	J/mol×K	639.73	Joback Method
cpg	484.22	J/mol×K	670.40	Joback Method
cpg	493.23	J/mol×K	701.07	Joback Method
cpg	501.53	J/mol×K	731.74	Joback Method
cpg	509.17	J/mol×K	762.41	Joback Method
cpg	516.19	J/mol×K	793.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375947&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