2-Chloro-4-fluorophenyl heptanfluorobutyrate

Inchi: InChI=1S/C10H3ClF8O2/c11-5-3-4(12)1-2-6(5)21-7(20)8(13,14)9(15,16)10(17,18)19/h1-
InchiKey: MPRBRTLOHUGHTL-UHFFFAOYSA-N
Formula: C10H3ClF8O2
SMILES: O=C(Oc1ccc(F)cc1Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 342.57

Physical Properties

Property code	Value	Unit	Source
gf	-1669.34	kJ/mol	Joback Method
hf	-1891.81	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.217		Crippen Method
mcvol	161.840	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1045.00		NIST Webbook
tb	563.03	K	Joback Method
tc	741.98	K	Joback Method
tf	367.98	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.25	J/mol×K	563.03	Joback Method
cpg	412.09	J/mol×K	592.85	Joback Method
cpg	421.14	J/mol×K	622.68	Joback Method
cpg	429.45	J/mol×K	652.50	Joback Method
cpg	437.07	J/mol×K	682.33	Joback Method
cpg	444.05	J/mol×K	712.15	Joback Method
cpg	450.42	J/mol×K	741.98	Joback Method

Sources

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=U373460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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