Heptafluorobutyric acid, 2-chlorophenyl ester

Inchi: InChI=1S/C10H4ClF7O2/c11-5-3-1-2-4-6(5)20-7(19)8(12,13)9(14,15)10(16,17)18/h1-4H
InchiKey: RTQMFWARAJJMNH-UHFFFAOYSA-N
Formula: C10H4ClF7O2
SMILES: O=C(Oc1ccccc1Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 324.58

Physical Properties

Property code	Value	Unit	Source
gf	-1464.90	kJ/mol	Joback Method
hf	-1684.23	kJ/mol	Joback Method
hfus	21.61	kJ/mol	Joback Method
hvap	44.73	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.078		Crippen Method
mcvol	160.070	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	558.78	K	Joback Method
tc	744.80	K	Joback Method
tf	354.87	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.61	J/mol×K	558.78	Joback Method
cpg	405.20	J/mol×K	589.78	Joback Method
cpg	414.91	J/mol×K	620.79	Joback Method
cpg	423.79	J/mol×K	651.79	Joback Method
cpg	431.90	J/mol×K	682.79	Joback Method
cpg	439.29	J/mol×K	713.80	Joback Method
cpg	446.02	J/mol×K	744.80	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299082&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume