2-Chloro-4-fluorophenyl pentafluoropropionate

Inchi: InChI=1S/C9H3ClF6O2/c10-5-3-4(11)1-2-6(5)18-7(17)8(12,13)9(14,15)16/h1-3H
InchiKey: JLZUYLPCKKBFCI-UHFFFAOYSA-N
Formula: C9H3ClF6O2
SMILES: O=C(Oc1ccc(F)cc1Cl)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 292.56

Physical Properties

Property code	Value	Unit	Source
gf	-1290.98	kJ/mol	Joback Method
hf	-1470.20	kJ/mol	Joback Method
hfus	22.96	kJ/mol	Joback Method
hvap	45.28	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.582		Crippen Method
mcvol	144.210	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1001.00		NIST Webbook
tb	544.84	K	Joback Method
tc	732.24	K	Joback Method
tf	353.11	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.41	J/mol×K	544.84	Joback Method
cpg	346.85	J/mol×K	576.07	Joback Method
cpg	355.59	J/mol×K	607.31	Joback Method
cpg	363.66	J/mol×K	638.54	Joback Method
cpg	371.09	J/mol×K	669.78	Joback Method
cpg	377.94	J/mol×K	701.01	Joback Method
cpg	384.22	J/mol×K	732.24	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=U373462&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

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