2-Chloro-4-fluoro-phenyl trifluoroacetate

Inchi: InChI=1S/C8H3ClF4O2/c9-5-3-4(10)1-2-6(5)15-7(14)8(11,12)13/h1-3H
InchiKey: DWZXRGYAJCHOGN-UHFFFAOYSA-N
Formula: C8H3ClF4O2
SMILES: O=C(Oc1ccc(F)cc1Cl)C(F)(F)F
Mol. weight [g/mol]: 242.56

Physical Properties

Property code	Value	Unit	Source
gf	-912.62	kJ/mol	Joback Method
hf	-1048.59	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.947		Crippen Method
mcvol	126.580	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
tb	526.65	K	Joback Method
tc	723.77	K	Joback Method
tf	338.24	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.03	J/mol×K	526.65	Joback Method
cpg	282.83	J/mol×K	559.50	Joback Method
cpg	291.05	J/mol×K	592.36	Joback Method
cpg	298.71	J/mol×K	625.21	Joback Method
cpg	305.83	J/mol×K	658.07	Joback Method
cpg	312.43	J/mol×K	690.92	Joback Method
cpg	318.53	J/mol×K	723.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373302&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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