Acetophenone, 4'-chloro-2,2-difluoro

Inchi: InChI=1S/C8H5ClF2O/c9-6-3-1-5(2-4-6)7(12)8(10)11/h1-4,8H
InchiKey: UVQWPRFEOFCDLY-UHFFFAOYSA-N
Formula: C8H5ClF2O
SMILES: O=C(c1ccc(Cl)cc1)C(F)F
Mol. weight [g/mol]: 190.57

Physical Properties

Property code	Value	Unit	Source
gf	-413.65	kJ/mol	Joback Method
hf	-509.21	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.788		Crippen Method
mcvol	117.170	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
tb	503.50	K	Joback Method
tc	713.93	K	Joback Method
tf	284.89	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.22	J/mol×K	503.50	Joback Method
cpg	243.06	J/mol×K	538.57	Joback Method
cpg	252.27	J/mol×K	573.64	Joback Method
cpg	260.86	J/mol×K	608.72	Joback Method
cpg	268.87	J/mol×K	643.79	Joback Method
cpg	276.30	J/mol×K	678.86	Joback Method
cpg	283.20	J/mol×K	713.93	Joback Method

Sources

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=R515003&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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