«alpha»-Chloro-p-fluoroacetophenone

Other names:	«alpha»-Chloro-para-fluoroacetophenone
	p-Fluoro-«alpha»-chloroacetophenone
	Ethanone, 2-chloro-1-(4-fluorophenyl)-
	Acetophenone, 2-chloro-4'-fluoro-
	p-Fluorophenacyl chloride
	2-Chloro-4'-fluoroacetophenone
	2-Chloro-1-(4-fluorophenyl)ethanone
	«alpha»-Chloro-4-fluoroacetophenone
Inchi:	InChI=1S/C8H6ClFO/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4H,5H2
InchiKey:	UJZWJOQRSMOFMA-UHFFFAOYSA-N
Formula:	C8H6ClFO
SMILES:	O=C(CCl)c1ccc(F)cc1
Mol. weight [g/mol]:	172.58
CAS:	456-04-2

Physical Properties

Property code	Value	Unit	Source
gf	-216.40	kJ/mol	Joback Method
hf	-307.82	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.247		Crippen Method
mcvol	115.400	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	504.67	K	Joback Method
tc	721.54	K	Joback Method
tf	299.30	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.55	J/mol×K	504.67	Joback Method

cpg	234.62	J/mol×K	540.82	Joback Method
cpg	244.03	J/mol×K	576.96	Joback Method
cpg	252.83	J/mol×K	613.11	Joback Method
cpg	261.03	J/mol×K	649.25	Joback Method
cpg	268.66	J/mol×K	685.40	Joback Method
cpg	275.74	J/mol×K	721.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C456042&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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