1-Butanone, 4-chloro-1-(4-fluorophenyl)-

Other names: «gamma»-Chloro-p-fluorobutyrophenone
3-Chloropropyl 4'-fluorophenyl ketone
«omega»-Chloro-4-fluorobutyrophenone
«gamma»-Chloro-4-fluorobutyrophenone
«omega»-Chloro-p-fluorobutyrophenone
p-Fluoro-«gamma»-chlorobutyrophenone
p-Fluoro-«omega»-chlorobutyrophenone
p-Fluoro-4-chlorobutyrophenone
p-Fluorobenzoylpropyl chloride
Butyrophenone, 4-chloro-4'-fluoro-
3-(p-Fluorobenzoyl)propyl chloride
3-(4-Fluorobenzoyl)propyl chloride
3-Chloro-4'-fluorobutyrophenone
3-Chloropropyl 4-fluorophenyl ketone
4-(p-Fluorophenyl)-4-oxobutyl chloride
4-(4-Fluorophenyl)-4-oxobutyl chloride
4-Chloro-p-fluorobutyrophenone
4-Chloro-4'-fluorobutyrophenone
4-Fluorobenzoylpropyl chloride
4'-Fluoro-4-chlorobutyrophenone
NSC 87082

Inchi: InChI=1S/C10H10ClFO/c11-7-1-2-10(13)8-3-5-9(12)6-4-8/h3-6H,1-2,7H2

InchiKey: HXAOUYGZEOZTJO-UHFFFAOYSA-N

Formula: C10H10ClFO

SMILES: O=C(CCCCl)c1ccc(F)cc1

Mol. weight [g/mol]: 200.64

CAS: 3874-54-2

Physical Properties

Property code	Value	Unit	Source
gf	-199.56	kJ/mol	Joback Method
hf	-349.10	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.027		Crippen Method

mcvol	143.580	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	550.43	K	Joback Method
tc	760.36	K	Joback Method
tf	321.84	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.95	J/mol×K	550.43	Joback Method
cpg	323.04	J/mol×K	585.42	Joback Method
cpg	334.40	J/mol×K	620.41	Joback Method
cpg	345.04	J/mol×K	655.40	Joback Method
cpg	354.99	J/mol×K	690.39	Joback Method
cpg	364.30	J/mol×K	725.38	Joback Method
cpg	372.99	J/mol×K	760.36	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3874542&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

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