Benzoyl chloride, 2-fluoro-

Other names:	o-Fluorobenzoyl chloride
	2-Fluorobenzoyl chloride
	ortho-Fluorobenzoyl chloride
	Benzoyl chloride, o-fluoro-
Inchi:	InChI=1S/C7H4ClFO/c8-7(10)5-3-1-2-4-6(5)9/h1-4H
InchiKey:	RAAGZOYMEQDCTD-UHFFFAOYSA-N
Formula:	C7H4ClFO
SMILES:	O=C(Cl)c1ccccc1F
Mol. weight [g/mol]:	158.56
CAS:	393-52-2

Physical Properties

Property code	Value	Unit	Source
gf	-224.82	kJ/mol	Joback Method
hf	-287.18	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.205		Crippen Method
mcvol	101.310	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	481.79	K	Joback Method
tc	702.19	K	Joback Method
tf	288.03	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.28	J/mol×K	481.79	Joback Method
cpg	193.11	J/mol×K	518.52	Joback Method
cpg	201.35	J/mol×K	555.26	Joback Method
cpg	209.03	J/mol×K	591.99	Joback Method
cpg	216.17	J/mol×K	628.72	Joback Method

cpg	222.79	J/mol×K	665.46	Joback Method
cpg	228.92	J/mol×K	702.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.00 ± 1.00	K	2.00	NIST Webbook
tbrp	364.00 ± 1.00	K	2.00	NIST Webbook
tbrp	364.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C393522&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume