2-Fluoro-4-(trifluoromethyl)benzoyl chloride

Inchi: InChI=1S/C8H3ClF4O/c9-7(14)5-2-1-4(3-6(5)10)8(11,12)13/h1-3H
InchiKey: OOAHPLWBUUTFMV-UHFFFAOYSA-N
Formula: C8H3ClF4O
SMILES: O=C(Cl)c1ccc(C(F)(F)F)cc1F
Mol. weight [g/mol]: 226.56
CAS: 126917-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-807.62	kJ/mol	Joback Method
hf	-916.37	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	43.57	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.224		Crippen Method
mcvol	120.710	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	504.23	K	Joback Method
tc	702.93	K	Joback Method
tf	316.01	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.84	J/mol×K	504.23	Joback Method
cpg	261.87	J/mol×K	537.35	Joback Method
cpg	270.24	J/mol×K	570.46	Joback Method
cpg	277.99	J/mol×K	603.58	Joback Method
cpg	285.15	J/mol×K	636.69	Joback Method
cpg	291.75	J/mol×K	669.81	Joback Method
cpg	297.83	J/mol×K	702.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126917100&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