3,5-Difluorobenzoyl chloride

Inchi: InChI=1S/C7H3ClF2O/c8-7(11)4-1-5(9)3-6(10)2-4/h1-3H
InchiKey: OYZWEOORLJBPMA-UHFFFAOYSA-N
Formula: C7H3ClF2O
SMILES: O=C(Cl)c1cc(F)cc(F)c1
Mol. weight [g/mol]: 176.55
CAS: 129714-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-429.26	kJ/mol	Joback Method
hf	-494.76	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	44.27	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.344		Crippen Method
mcvol	103.080	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	486.04	K	Joback Method
tc	696.07	K	Joback Method
tf	301.14	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.28	J/mol×K	486.04	Joback Method
cpg	200.24	J/mol×K	521.04	Joback Method
cpg	207.73	J/mol×K	556.05	Joback Method
cpg	214.74	J/mol×K	591.05	Joback Method
cpg	221.31	J/mol×K	626.06	Joback Method
cpg	227.44	J/mol×K	661.06	Joback Method
cpg	233.14	J/mol×K	696.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129714972&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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