2,4,6-Trifluorobenzoyl chloride

Inchi: InChI=1S/C7H2ClF3O/c8-7(12)6-4(10)1-3(9)2-5(6)11/h1-2H
InchiKey: SIFIJQFBERMWMU-UHFFFAOYSA-N
Formula: C8H5F3O
SMILES: O=C(Cl)c1c(F)cc(F)cc1F
Mol. weight [g/mol]: 174.12
CAS: 79538-29-7

Physical Properties

Property code	Value	Unit	Source
gf	-633.70	kJ/mol	Joback Method
hf	-702.34	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	44.12	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.483		Crippen Method
mcvol	104.850	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	490.29	K	Joback Method
tc	690.73	K	Joback Method
tf	314.25	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.18	J/mol×K	490.29	Joback Method
cpg	207.35	J/mol×K	523.70	Joback Method
cpg	214.14	J/mol×K	557.10	Joback Method
cpg	220.54	J/mol×K	590.51	Joback Method
cpg	226.57	J/mol×K	623.92	Joback Method
cpg	232.24	J/mol×K	657.33	Joback Method
cpg	237.54	J/mol×K	690.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79538297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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