3-Chlorophenol, trifluoroacetate

Inchi: InChI=1S/C8H4ClF3O2/c9-5-2-1-3-6(4-5)14-7(13)8(10,11)12/h1-4H
InchiKey: IVGWAFXWYCCNGV-UHFFFAOYSA-N
Formula: C8H4ClF3O2
SMILES: O=C(Oc1cccc(Cl)c1)C(F)(F)F
Mol. weight [g/mol]: 224.56

Physical Properties

Property code	Value	Unit	Source
gf	-708.18	kJ/mol	Joback Method
hf	-841.01	kJ/mol	Joback Method
hfus	18.94	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.808		Crippen Method
mcvol	124.810	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1016.00		NIST Webbook
tb	522.40	K	Joback Method
tc	728.51	K	Joback Method
tf	325.13	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.30	J/mol×K	522.40	Joback Method
cpg	275.92	J/mol×K	556.75	Joback Method
cpg	284.85	J/mol×K	591.10	Joback Method
cpg	293.13	J/mol×K	625.46	Joback Method
cpg	300.78	J/mol×K	659.81	Joback Method
cpg	307.83	J/mol×K	694.16	Joback Method
cpg	314.32	J/mol×K	728.51	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=U374282&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume