2,3,5-Trichlorophenol, O-trifluoroacetyl-

Inchi: InChI=1S/C8H2Cl3F3O2/c9-3-1-4(10)6(11)5(2-3)16-7(15)8(12,13)14/h1-2H
InchiKey: VRHGAJDZCAFIGN-UHFFFAOYSA-N
Formula: C8H2Cl3F3O2
SMILES: O=C(Oc1cc(Cl)cc(Cl)c1Cl)C(F)(F)F
Mol. weight [g/mol]: 293.45

Physical Properties

Property code	Value	Unit	Source
gf	-751.30	kJ/mol	Joback Method
hf	-895.43	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.115		Crippen Method
mcvol	149.290	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
tb	607.22	K	Joback Method
tc	823.97	K	Joback Method
tf	410.01	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.46	J/mol×K	607.22	Joback Method
cpg	313.90	J/mol×K	643.35	Joback Method
cpg	320.74	J/mol×K	679.47	Joback Method
cpg	327.02	J/mol×K	715.60	Joback Method
cpg	332.75	J/mol×K	751.72	Joback Method
cpg	337.96	J/mol×K	787.85	Joback Method
cpg	342.68	J/mol×K	823.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374269&Units=SI

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