2,6-Dichlorophenol, trifluoroacetate

Inchi: InChI=1S/C8H3Cl2F3O2/c9-4-2-1-3-5(10)6(4)15-7(14)8(11,12)13/h1-3H
InchiKey: OBHNRRCJWQZHDD-UHFFFAOYSA-N
Formula: C8H3Cl2F3O2
SMILES: O=C(Oc1c(Cl)cccc1Cl)C(F)(F)F
Mol. weight [g/mol]: 259.01

Physical Properties

Property code	Value	Unit	Source
gf	-729.74	kJ/mol	Joback Method
hf	-868.22	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	51.18	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.461		Crippen Method
mcvol	137.050	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	564.81	K	Joback Method
tc	776.60	K	Joback Method
tf	367.57	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.51	J/mol×K	564.81	Joback Method
cpg	296.00	J/mol×K	600.11	Joback Method
cpg	303.86	J/mol×K	635.41	Joback Method
cpg	311.11	J/mol×K	670.70	Joback Method
cpg	317.77	J/mol×K	706.00	Joback Method
cpg	323.87	J/mol×K	741.30	Joback Method
cpg	329.45	J/mol×K	776.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374856&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume