Trichloroacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C8H5Cl3FNO/c9-8(10,11)7(14)13-6-4-2-1-3-5(6)12/h1-4H,(H,13,14)
InchiKey: CICMDDPELVRHCE-UHFFFAOYSA-N
Formula: C8H5Cl3FNO
SMILES: O=C(Nc1ccccc1F)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 256.49

Physical Properties

Property code	Value	Unit	Source
gf	-148.03	kJ/mol	Joback Method
hf	-294.58	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.134		Crippen Method
mcvol	149.860	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
tb	626.47	K	Joback Method
tc	865.04	K	Joback Method
tf	414.22	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.27	J/mol×K	626.47	Joback Method
cpg	322.17	J/mol×K	666.23	Joback Method
cpg	330.21	J/mol×K	705.99	Joback Method
cpg	337.45	J/mol×K	745.76	Joback Method
cpg	343.98	J/mol×K	785.52	Joback Method
cpg	349.85	J/mol×K	825.28	Joback Method
cpg	355.14	J/mol×K	865.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308484&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