N-(2,3,5,6-Tetrachlorophenyl)-2,2,3,3,3-pentafluor

Other names: 2,3,5,6-Tetrachloroaniline, pentafluoropropionate
Inchi: InChI=1S/C9H2Cl4F5NO/c10-2-1-3(11)5(13)6(4(2)12)19-7(20)8(14,15)9(16,17)18/h1H,(H
InchiKey: KMEILKVHKGJFIF-UHFFFAOYSA-N
Formula: C9H2Cl4F5NO
SMILES: O=C(Nc1c(Cl)c(Cl)cc(Cl)c1Cl)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 376.92

Physical Properties

Property code	Value	Unit	Source
gf	-956.83	kJ/mol	Joback Method
hf	-1158.56	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.436		Crippen Method
mcvol	183.270	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	695.57	K	Joback Method
tc	907.52	K	Joback Method
tf	497.75	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.82	J/mol×K	695.57	Joback Method
cpg	416.46	J/mol×K	730.90	Joback Method
cpg	422.46	J/mol×K	766.22	Joback Method
cpg	427.87	J/mol×K	801.55	Joback Method
cpg	432.75	J/mol×K	836.87	Joback Method
cpg	437.17	J/mol×K	872.20	Joback Method
cpg	441.19	J/mol×K	907.52	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=U373424&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