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

Other names: 2,3,5,6-Tetrachloroaniline, N-trifluoroacetyl
Inchi: InChI=1S/C8H2Cl4F3NO/c9-2-1-3(10)5(12)6(4(2)11)16-7(17)8(13,14)15/h1H,(H,16,17)
InchiKey: DFFXCENOFFIGME-UHFFFAOYSA-N
Formula: C8H2Cl4F3NO
SMILES: O=C(Nc1c(Cl)c(Cl)cc(Cl)c1Cl)C(F)(F)F
Mol. weight [g/mol]: 326.92

Physical Properties

Property code	Value	Unit	Source
gf	-578.47	kJ/mol	Joback Method
hf	-736.95	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	65.30	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.801		Crippen Method
mcvol	165.640	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1658.00		NIST Webbook
tb	677.38	K	Joback Method
tc	900.00	K	Joback Method
tf	482.88	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.09	J/mol×K	677.38	Joback Method
cpg	349.61	J/mol×K	714.48	Joback Method
cpg	355.53	J/mol×K	751.59	Joback Method
cpg	360.91	J/mol×K	788.69	Joback Method
cpg	365.77	J/mol×K	825.79	Joback Method
cpg	370.17	J/mol×K	862.90	Joback Method
cpg	374.14	J/mol×K	900.00	Joback Method

Sources

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=U373259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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