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

Other names: 2,3,5,6-Tetrachloroaniline, bis(trifluoroacetate)
Inchi: InChI=1S/C10HCl4F6NO2/c11-2-1-3(12)5(14)6(4(2)13)21(7(22)9(15,16)17)8(23)10(18,1
InchiKey: GTTNRIZDDVRIDP-UHFFFAOYSA-N
Formula: C10HCl4F6NO2
SMILES: O=C(N(C(=O)C(F)(F)F)c1c(Cl)c(Cl)cc(Cl)c1Cl)C(F)(F)F
Mol. weight [g/mol]: 422.92

Physical Properties

Property code	Value	Unit	Source
gf	-1250.75	kJ/mol	Joback Method
hf	-1473.83	kJ/mol	Joback Method
hfus	40.80	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.284		Crippen Method
mcvol	200.700	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	733.86	K	Joback Method
tc	939.04	K	Joback Method
tf	539.35	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.33	J/mol×K	733.86	Joback Method
cpg	470.50	J/mol×K	768.06	Joback Method
cpg	476.05	J/mol×K	802.25	Joback Method
cpg	481.03	J/mol×K	836.45	Joback Method
cpg	485.51	J/mol×K	870.65	Joback Method
cpg	489.56	J/mol×K	904.84	Joback Method
cpg	493.23	J/mol×K	939.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373257&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

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