N-(2,3,5,6-Tetrachlorophenyl)-2,2,3,3,4,4,4-heptafl

Other names: 2,3,5,6-Tetrachloroaniline, N-heptanfluorobutyryl-
Inchi: InChI=1S/C10H2Cl4F7NO/c11-2-1-3(12)5(14)6(4(2)13)22-7(23)8(15,16)9(17,18)10(19,2
InchiKey: SKPPZZKSFHCXOB-UHFFFAOYSA-N
Formula: C10H2Cl4F7NO
SMILES: O=C(Nc1c(Cl)c(Cl)cc(Cl)c1Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 426.93

Physical Properties

Property code	Value	Unit	Source
gf	-1335.19	kJ/mol	Joback Method
hf	-1580.17	kJ/mol	Joback Method
hfus	36.94	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.072		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1702.00		NIST Webbook
tb	713.76	K	Joback Method
tc	916.74	K	Joback Method
tf	512.62	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.17	J/mol×K	713.76	Joback Method
cpg	483.82	J/mol×K	747.59	Joback Method
cpg	489.81	J/mol×K	781.42	Joback Method
cpg	495.20	J/mol×K	815.25	Joback Method
cpg	500.07	J/mol×K	849.08	Joback Method
cpg	504.50	J/mol×K	882.91	Joback Method
cpg	508.55	J/mol×K	916.74	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=U373258&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