N,N-Diphenylcarbamic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C19H11Cl4NO2/c20-14-11-15(21)18(17(23)16(14)22)26-19(25)24(12-7-3-1-4-8

InchiKey: KXDCOQMCUIBZCZ-UHFFFAOYSA-N

Formula: C19H11Cl4NO2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)N(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 427.11

Physical Properties

Property code	Value	Unit	Source
gf	236.95	kJ/mol	Joback Method
hf	-12.01	kJ/mol	Joback Method
hfus	48.13	kJ/mol	Joback Method
hvap	96.10	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.637		Crippen Method
mcvol	273.670	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	972.53	K	Joback Method
tc	1238.98	K	Joback Method
tf	657.54	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.77	J/mol×K	972.53	Joback Method
cpg	713.73	J/mol×K	1016.94	Joback Method
cpg	721.57	J/mol×K	1061.35	Joback Method
cpg	728.38	J/mol×K	1105.76	Joback Method
cpg	734.29	J/mol×K	1150.16	Joback Method
cpg	739.38	J/mol×K	1194.57	Joback Method
cpg	743.77	J/mol×K	1238.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360536&Units=SI

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