N,N-Diphenylcarbamic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C19H12Cl3NO2/c20-15-11-17(22)18(12-16(15)21)25-19(24)23(13-7-3-1-4-8-13

InchiKey: FRZWCDXDXOIWPL-UHFFFAOYSA-N

Formula: C19H12Cl3NO2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)N(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 392.66

Physical Properties

Property code	Value	Unit	Source
gf	258.51	kJ/mol	Joback Method
hf	15.20	kJ/mol	Joback Method
hfus	44.32	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.984		Crippen Method
mcvol	261.430	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	930.12	K	Joback Method
tc	1194.39	K	Joback Method
tf	615.10	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.33	J/mol×K	930.12	Joback Method
cpg	699.70	J/mol×K	974.16	Joback Method
cpg	708.87	J/mol×K	1018.21	Joback Method
cpg	716.94	J/mol×K	1062.25	Joback Method
cpg	724.02	J/mol×K	1106.30	Joback Method
cpg	730.23	J/mol×K	1150.34	Joback Method
cpg	735.67	J/mol×K	1194.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360535&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

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