N,N-Diphenylcarbamic acid, pentafluorophenyl ester

Inchi: InChI=1S/C19H10F5NO2/c20-13-14(21)16(23)18(17(24)15(13)22)27-19(26)25(11-7-3-1-
InchiKey: BXCZUQHKRKEAIU-UHFFFAOYSA-N
Formula: C19H10F5NO2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 379.28

Physical Properties

Property code	Value	Unit	Source
gf	-699.01	kJ/mol	Joback Method
hf	-941.07	kJ/mol	Joback Method
hfus	46.35	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	5.719		Crippen Method
mcvol	233.560	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	824.14	K	Joback Method
tc	1041.16	K	Joback Method
tf	553.33	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.49	J/mol×K	824.14	Joback Method
cpg	674.12	J/mol×K	860.31	Joback Method
cpg	684.71	J/mol×K	896.48	Joback Method
cpg	694.30	J/mol×K	932.65	Joback Method
cpg	702.95	J/mol×K	968.82	Joback Method
cpg	710.70	J/mol×K	1004.99	Joback Method
cpg	717.59	J/mol×K	1041.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360534&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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