N,N-Diphenylcarbamic acid, 4-biphenyl ester

Inchi: InChI=1S/C25H19NO2/c27-25(26(22-12-6-2-7-13-22)23-14-8-3-9-15-23)28-24-18-16-21(
InchiKey: AEYFPYAZOWKZRY-UHFFFAOYSA-N
Formula: C25H19NO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	476.49	kJ/mol	Joback Method
hf	198.05	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.691		Crippen Method
mcvol	285.490	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	971.83	K	Joback Method
tc	1240.95	K	Joback Method
tf	594.34	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.94	J/mol×K	971.83	Joback Method
cpg	882.31	J/mol×K	1016.68	Joback Method
cpg	894.27	J/mol×K	1061.54	Joback Method
cpg	905.01	J/mol×K	1106.39	Joback Method
cpg	914.70	J/mol×K	1151.24	Joback Method
cpg	923.54	J/mol×K	1196.10	Joback Method
cpg	931.71	J/mol×K	1240.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360537&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