4,4'-Dianilino-3,3'-diaminodiphenyl oxide

Inchi: InChI=1S/C24H22N4O/c25-21-15-19(11-13-23(21)27-17-7-3-1-4-8-17)29-20-12-14-24(22
InchiKey: CVFQPTVXHUGUJS-UHFFFAOYSA-N
Formula: C24H22N4O
SMILES: Nc1cc(Oc2ccc(Nc3ccccc3)c(N)c2)ccc1Nc1ccccc1
Mol. weight [g/mol]: 382.46
CAS: 18888-98-7

Physical Properties

Property code	Value	Unit	Source
gf	769.00	kJ/mol	Joback Method
hf	403.85	kJ/mol	Joback Method
hfus	54.30	kJ/mol	Joback Method
hvap	117.33	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	6.130		Crippen Method
mcvol	299.770	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	1142.98	K	Joback Method
tc	1421.35	K	Joback Method
tf	810.07	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.82	J/mol×K	1142.98	Joback Method
cpg	982.05	J/mol×K	1189.38	Joback Method
cpg	990.14	J/mol×K	1235.77	Joback Method
cpg	997.24	J/mol×K	1282.17	Joback Method
cpg	1003.52	J/mol×K	1328.56	Joback Method
cpg	1009.12	J/mol×K	1374.96	Joback Method
cpg	1014.22	J/mol×K	1421.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18888987&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume