

2,5-Bis (n-benzyl-n-methyl-aminomethyl) hydroquinone

Inchi:	InChI=1S/C24H28N2O2/c1-25(15-19-9-5-3-6-10-19)17-21-13-24(28)22(14-23(21)27)18-2
InchiKey:	DGMRPOQWQUAUKE-UHFFFAOYSA-N
Formula:	C24H28N2O2
SMILES:	CN(Cc1ccccc1)Cc1cc(O)c(CN(C)Cc2ccccc2)cc1O
Mol. weight [g/mol]:	376.49
CAS:	96668-33-6

Physical Properties

Property code	Value	Unit	Source
gf	391.12	kJ/mol	Joback Method
hf	-60.13	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	106.62	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.362		Crippen Method
mcvol	309.440	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
tb	1019.66	K	Joback Method
tc	1268.07	K	Joback Method
tf	740.40	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.69	J/molxK	1019.66	Joback Method
cpg	1047.44	J/molxK	1061.06	Joback Method
cpg	1066.46	J/molxK	1102.46	Joback Method
cpg	1086.02	J/molxK	1143.86	Joback Method
cpg	1106.42	J/molxK	1185.27	Joback Method
cpg	1127.93	J/molxK	1226.67	Joback Method
cpg	1150.85	J/molxK	1268.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C96668336&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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