

Alpha,alpha'-bis(dimethylamino)-4,4'-di-o-cresol

Inchi:	InChI=1S/C18H24N2O2/c1-19(2)11-15-9-13(5-7-17(15)21)14-6-8-18(22)16(10-14)12-20
InchiKey:	ZQVLGUNSVGXEGL-UHFFFAOYSA-N
Formula:	C18H24N2O2
SMILES:	CN(C)Cc1cc(-c2ccc(O)c(CN(C)C)c2)ccc1O
Mol. weight [g/mol]:	300.40
CAS:	10554-73-1

Physical Properties

Property code	Value	Unit	Source
gf	218.56	kJ/mol	Joback Method
hf	-184.29	kJ/mol	Joback Method
hfus	47.29	kJ/mol	Joback Method
hvap	91.65	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.888		Crippen Method
mcvol	248.660	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	860.68	K	Joback Method
tc	1093.07	K	Joback Method
tf	658.88	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.70	J/molxK	860.68	Joback Method
cpg	786.45	J/molxK	899.41	Joback Method
cpg	801.76	J/molxK	938.14	Joback Method
cpg	816.80	J/molxK	976.88	Joback Method
cpg	831.77	J/molxK	1015.61	Joback Method
cpg	846.86	J/molxK	1054.34	Joback Method
cpg	862.26	J/molxK	1093.07	Joback Method

Sources

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=C10554731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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