

Alpha,alpha'-bis(2-tert-butyl-anilino)-p-xylene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C28H36N2/c1-27(2,3)23-11-7-9-13-25(23)29-19-21-15-17-22(18-16-21)20-30-7

LBNZFAPCYWYTAU-UHFFFAOYSA-N

C28H36N2

CC(C)(C)c1ccccc1NCc1ccc(CNc2ccccc2C(C)(C)C)cc1

400.60

Physical Properties

Property code	Value	Unit	Source
gf	677.68	kJ/mol	Joback Method
hf	143.37	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	97.02	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.506		Crippen Method
mcvol	354.060	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
tb	1028.90	K	Joback Method
tc	1276.40	K	Joback Method
tf	632.30	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.69	J/mol×K	1028.90	Joback Method
cpg	1206.04	J/mol×K	1070.15	Joback Method
cpg	1222.50	J/mol×K	1111.40	Joback Method
cpg	1238.26	J/mol×K	1152.65	Joback Method
cpg	1253.53	J/mol×K	1193.90	Joback Method
cpg	1268.52	J/mol×K	1235.15	Joback Method
cpg	1283.43	J/mol×K	1276.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=B6008508&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
mcvol:	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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