

Propane, 1,3-bis(2-tert-butyl-4-methylanilino)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H38N2/c1-18-10-12-22(20(16-18)24(3,4)5)26-14-9-15-27-23-13-11-19(2)1

CKUWUFOAHQTZOE-UHFFFAOYSA-N

C25H38N2

Cc1ccc(NCCCNc2ccc(C)cc2C(C)(C)C)c(C(C)(C)C)c1

366.58

Physical Properties

Property code	Value	Unit	Source
gf	530.38	kJ/mol	Joback Method
hf	-42.71	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.813		Crippen Method
mcvol	335.550	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
tb	938.56	K	Joback Method
tc	1164.97	K	Joback Method
tf	584.59	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.35	J/mol×K	938.56	Joback Method
cpg	1125.67	J/mol×K	976.29	Joback Method
cpg	1142.88	J/mol×K	1014.03	Joback Method
cpg	1159.09	J/mol×K	1051.76	Joback Method
cpg	1174.45	J/mol×K	1089.50	Joback Method
cpg	1189.08	J/mol×K	1127.23	Joback Method
cpg	1203.11	J/mol×K	1164.97	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=B6008505&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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