

Bis-(4-amino-5-tert-butyl-3-methylphenyl)methane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C23H34N2/c1-14-9-16(12-18(20(14)24)22(3,4)5)11-17-10-15(2)21(25)19(13-1

WGXCShNHXHXHBS-UHFFFAOYSA-N

C23H34N2

Cc1cc(Cc2cc(C)c(N)c(C(C)(C)C)c2)cc(C(C)(C)C)c1N

338.53

13680-36-9

Physical Properties

Property code	Value	Unit	Source
gf	448.40	kJ/mol	Joback Method
hf	-63.73	kJ/mol	Joback Method
hfus	36.64	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.654		Crippen Method
mcvol	307.370	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
tb	947.48	K	Joback Method
tc	1189.17	K	Joback Method
tf	648.29	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.36	J/mol×K	947.48	Joback Method
cpg	1020.52	J/mol×K	987.76	Joback Method
cpg	1036.56	J/mol×K	1028.04	Joback Method
cpg	1051.63	J/mol×K	1068.33	Joback Method
cpg	1065.86	J/mol×K	1108.61	Joback Method
cpg	1079.37	J/mol×K	1148.89	Joback Method
cpg	1092.29	J/mol×K	1189.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13680369&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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