

P-tert-amyl-n,n-bis(3-phenylpropyl)aniline

Inchi:	InChI=1S/C29H37N/c1-4-29(2,3)27-19-21-28(22-20-27)30(23-11-17-25-13-7-5-8-14-25)2
InchiKey:	IHBUEIMCUVOJL-UHFFFAOYSA-N
Formula:	C29H37N
SMILES:	CCC(C)(C)c1ccc(N(CCCc2ccccc2)CCc2ccccc2)cc1
Mol. weight [g/mol]:	399.61
CAS:	116436-27-2

Physical Properties

Property code	Value	Unit	Source
gf	634.52	kJ/mol	Joback Method
hf	115.01	kJ/mol	Joback Method
hfus	48.21	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.446		Crippen Method
mvol	358.170	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
tb	957.15	K	Joback Method
tc	1190.20	K	Joback Method
tf	543.26	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.59	J/molxK	957.15	Joback Method
cpg	1194.47	J/molxK	995.99	Joback Method
cpg	1212.18	J/molxK	1034.83	Joback Method
cpg	1228.90	J/molxK	1073.67	Joback Method
cpg	1244.81	J/molxK	1112.51	Joback Method
cpg	1260.07	J/molxK	1151.36	Joback Method
cpg	1274.86	J/molxK	1190.20	Joback Method

Sources

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=C116436272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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