N-tert-Butyl-N'-(4-ethylbenzoyl)-3,5-dimethylbenzo

Inchi: InChI=1S/C22H28N2O2/c1-7-17-8-10-18(11-9-17)20(25)23-24(22(4,5)6)21(26)19-13-15(

InchiKey: QYPNKSZPJQQLRK-UHFFFAOYSA-N

Formula: C22H28N2O2

SMILES: CCc1ccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)cc1

Mol. weight [g/mol]: 352.48

Physical Properties

Property code	Value	Unit	Source
gf	275.46	kJ/mol	Joback Method
hf	-171.67	kJ/mol	Joback Method
hfus	43.55	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-5.63		Aqueous Solubility Prediction Method
logp	4.452		Crippen Method
mcvol	296.420	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
tb	938.18	K	Joback Method
tc	1169.56	K	Joback Method
tf	615.51	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.33	J/mol×K	938.18	Joback Method
cpg	954.17	J/mol×K	976.74	Joback Method
cpg	967.91	J/mol×K	1015.31	Joback Method
cpg	980.68	J/mol×K	1053.87	Joback Method
cpg	992.59	J/mol×K	1092.43	Joback Method
cpg	1003.74	J/mol×K	1131.00	Joback Method
cpg	1014.25	J/mol×K	1169.56	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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