4-Tert-butyl-2-[(dibutylamino)methyl]phenol

Inchi: InChI=1S/C19H33NO/c1-6-8-12-20(13-9-7-2)15-16-14-17(19(3,4)5)10-11-18(16)21/h10-1
InchiKey: FRWBPYRXGBSUKA-UHFFFAOYSA-N
Formula: C19H33NO
SMILES: CCCCN(CCCC)Cc1cc(C(C)(C)C)ccc1O
Mol. weight [g/mol]: 291.47
CAS: 25544-02-9

Physical Properties

Property code	Value	Unit	Source
gf	170.88	kJ/mol	Joback Method
hf	-328.96	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	74.59	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	5.092		Crippen Method
mcvol	270.660	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
tb	755.61	K	Joback Method
tc	956.82	K	Joback Method
tf	489.44	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.39	J/mol×K	755.61	Joback Method
cpg	840.98	J/mol×K	789.14	Joback Method
cpg	858.61	J/mol×K	822.68	Joback Method
cpg	875.37	J/mol×K	856.21	Joback Method
cpg	891.38	J/mol×K	889.75	Joback Method
cpg	906.72	J/mol×K	923.28	Joback Method
cpg	921.51	J/mol×K	956.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25544029&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