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

Inchi: InChI=1S/C15H25NO/c1-6-16(7-2)11-12-10-13(15(3,4)5)8-9-14(12)17/h8-10,17H,6-7,11H
InchiKey: QDWJJXLKCWAPHS-UHFFFAOYSA-N
Formula: C15H25NO
SMILES: CCN(CC)Cc1cc(C(C)(C)C)ccc1O
Mol. weight [g/mol]: 235.37
CAS: 20484-34-8

Physical Properties

Property code	Value	Unit	Source
gf	137.20	kJ/mol	Joback Method
hf	-246.40	kJ/mol	Joback Method
hfus	29.65	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.532		Crippen Method
mcvol	214.300	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	664.09	K	Joback Method
tc	874.83	K	Joback Method
tf	444.36	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.18	J/mol×K	664.09	Joback Method
cpg	616.69	J/mol×K	699.21	Joback Method
cpg	633.12	J/mol×K	734.34	Joback Method
cpg	648.58	J/mol×K	769.46	Joback Method
cpg	663.18	J/mol×K	804.58	Joback Method
cpg	677.02	J/mol×K	839.70	Joback Method
cpg	690.21	J/mol×K	874.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20484348&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