3-Tert-butyl-4-(dimethylamino)phenol

Inchi: InChI=1S/C12H19NO/c1-12(2,3)10-8-9(14)6-7-11(10)13(4)5/h6-8,14H,1-5H3
InchiKey: JBSVDFYRJWPKER-UHFFFAOYSA-N
Formula: C12H19NO
SMILES: CN(C)c1ccc(O)cc1C(C)(C)C
Mol. weight [g/mol]: 193.29
CAS: 24197-40-8

Physical Properties

Property code	Value	Unit	Source
gf	111.94	kJ/mol	Joback Method
hf	-184.48	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	59.01	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.756		Crippen Method
mcvol	172.030	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	595.45	K	Joback Method
tc	817.19	K	Joback Method
tf	410.55	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.80	J/mol×K	595.45	Joback Method
cpg	461.10	J/mol×K	632.41	Joback Method
cpg	476.25	J/mol×K	669.36	Joback Method
cpg	490.36	J/mol×K	706.32	Joback Method
cpg	503.54	J/mol×K	743.28	Joback Method
cpg	515.90	J/mol×K	780.23	Joback Method
cpg	527.56	J/mol×K	817.19	Joback Method

Sources

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=C24197408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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