4-tert-Butylphenol, isoBOC

Inchi: InChI=1S/C15H22O3/c1-11(2)10-17-14(16)18-13-8-6-12(7-9-13)15(3,4)5/h6-9,11H,10H2
InchiKey: FEAHIYSSAKYIDE-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CC(C)COC(=O)Oc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-160.32	kJ/mol	Joback Method
hf	-518.92	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	61.80	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.155		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1727.00		NIST Webbook
tb	669.30	K	Joback Method
tc	879.92	K	Joback Method
tf	379.56	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.18	J/mol×K	669.30	Joback Method
cpg	594.37	J/mol×K	704.40	Joback Method
cpg	610.49	J/mol×K	739.51	Joback Method
cpg	625.57	J/mol×K	774.61	Joback Method
cpg	639.64	J/mol×K	809.71	Joback Method
cpg	652.73	J/mol×K	844.82	Joback Method
cpg	664.87	J/mol×K	879.92	Joback Method
dvisc	0.0014048	Pa×s	379.56	Joback Method
dvisc	0.0006732	Pa×s	427.85	Joback Method

dvisc	0.0003745	Pa×s	476.14	Joback Method
dvisc	0.0002321	Pa×s	524.43	Joback Method
dvisc	0.0001560	Pa×s	572.72	Joback Method
dvisc	0.0001115	Pa×s	621.01	Joback Method
dvisc	0.0000836	Pa×s	669.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235262&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume