4-tert-butyl-2-sec-butylphenol

Inchi: InChI=1S/C14H22O/c1-6-10(2)12-9-11(14(3,4)5)7-8-13(12)15/h7-10,15H,6H2,1-5H3
InchiKey: JKFZLMPBXBMSPD-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CCC(C)c1cc(C(C)(C)C)ccc1O
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	15.56	kJ/mol	Joback Method
hf	-298.57	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.203		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1590.00		NIST Webbook
tb	628.33	K	Joback Method
tc	849.96	K	Joback Method
tf	385.62	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.53	J/mol×K	628.33	Joback Method
cpg	584.82	J/mol×K	813.02	Joback Method
cpg	571.39	J/mol×K	776.09	Joback Method
cpg	557.15	J/mol×K	739.15	Joback Method
cpg	542.00	J/mol×K	702.21	Joback Method
cpg	525.83	J/mol×K	665.27	Joback Method
cpg	597.57	J/mol×K	849.96	Joback Method
dvisc	0.0000194	Pa×s	628.33	Joback Method
dvisc	0.0000314	Pa×s	587.88	Joback Method

dvisc	0.0000546	Pa×s	547.43	Joback Method
dvisc	0.0001037	Pa×s	506.98	Joback Method
dvisc	0.0002202	Pa×s	466.52	Joback Method
dvisc	0.0005394	Pa×s	426.07	Joback Method
dvisc	0.0015945	Pa×s	385.62	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=R169898&Units=SI

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