4-methyl-2-tert-butyl-6-hydroxym ethyl-phenol

Inchi: InChI=1S/C12H18O2/c1-8-5-9(7-13)11(14)10(6-8)12(2,3)4/h5-6,13-14H,7H2,1-4H3
InchiKey: OVXVAICEGAXQFZ-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: Cc1cc(CO)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-145.29	kJ/mol	Joback Method
hf	-415.71	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.490		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1544.00		NIST Webbook
tb	680.17	K	Joback Method
tc	889.74	K	Joback Method
tf	451.42	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.65	J/mol×K	680.17	Joback Method
cpg	474.12	J/mol×K	715.10	Joback Method
cpg	485.87	J/mol×K	750.03	Joback Method
cpg	496.98	J/mol×K	784.96	Joback Method
cpg	507.55	J/mol×K	819.89	Joback Method
cpg	517.64	J/mol×K	854.81	Joback Method
cpg	527.34	J/mol×K	889.74	Joback Method
dvisc	0.0003777	Pa×s	451.42	Joback Method
dvisc	0.0001378	Pa×s	489.54	Joback Method

dvisc	0.0000582	Pa×s	527.67	Joback Method
dvisc	0.0000276	Pa×s	565.79	Joback Method
dvisc	0.0000144	Pa×s	603.92	Joback Method
dvisc	0.0000081	Pa×s	642.04	Joback Method
dvisc	0.0000049	Pa×s	680.17	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=R169863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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