4-sec-Butyl-2-tert-butyl-6-hydroxymethyl-phenol

Inchi: InChI=1S/C15H24O2/c1-6-10(2)11-7-12(9-16)14(17)13(8-11)15(3,4)5/h7-8,10,16-17H,6,9

InchiKey: YSDSUIRQJMIZFL-UHFFFAOYSA-N

Formula: C15H24O2

SMILES: CCC(C)c1cc(CO)c(O)c(C(C)(C)C)c1

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-122.47	kJ/mol	Joback Method
hf	-482.91	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	80.59	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.696		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	748.37	K	Joback Method
tc	953.80	K	Joback Method
tf	470.23	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.19	J/mol×K	748.37	Joback Method
cpg	634.48	J/mol×K	782.61	Joback Method
cpg	648.03	J/mol×K	816.85	Joback Method
cpg	660.94	J/mol×K	851.08	Joback Method
cpg	673.29	J/mol×K	885.32	Joback Method
cpg	685.16	J/mol×K	919.56	Joback Method
cpg	696.64	J/mol×K	953.80	Joback Method
dvisc	0.0002604	Pa×s	470.23	Joback Method
dvisc	0.0000803	Pa×s	516.59	Joback Method

dvisc	0.0000301	Pa×s	562.94	Joback Method
dvisc	0.0000131	Pa×s	609.30	Joback Method
dvisc	0.0000064	Pa×s	655.66	Joback Method
dvisc	0.0000034	Pa×s	702.01	Joback Method
dvisc	0.0000020	Pa×s	748.37	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=R169883&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