2,4-Dibutylphenol

Inchi: InChI=1S/C14H22O/c1-3-5-7-12-9-10-14(15)13(11-12)8-6-4-2/h9-11,15H,3-8H2,1-2H3
InchiKey: KPZBEZVZFBDKCG-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CCCCc1ccc(O)c(CCCC)c1
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	15.16	kJ/mol	Joback Method
hf	-284.54	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.077		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
tb	632.00	K	Joback Method
tc	837.52	K	Joback Method
tf	398.20	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.06	J/mol×K	632.00	Joback Method
cpg	577.58	J/mol×K	803.27	Joback Method
cpg	564.58	J/mol×K	769.02	Joback Method
cpg	550.90	J/mol×K	734.76	Joback Method
cpg	536.47	J/mol×K	700.51	Joback Method
cpg	521.21	J/mol×K	666.25	Joback Method
cpg	589.96	J/mol×K	837.52	Joback Method
dvisc	0.0000234	Pa×s	632.00	Joback Method

dvisc	0.0000359	Pa×s	593.03	Joback Method
dvisc	0.0000585	Pa×s	554.07	Joback Method
dvisc	0.0001028	Pa×s	515.10	Joback Method
dvisc	0.0001979	Pa×s	476.13	Joback Method
dvisc	0.0004282	Pa×s	437.17	Joback Method
dvisc	0.0010778	Pa×s	398.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R266598&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