5-Methyl-2,4-diisopropylphenol

Other names: Phenol, 5-methyl-2,4-diisopropyl
Inchi: InChI=1S/C13H20O/c1-8(2)11-7-12(9(3)4)13(14)6-10(11)5/h6-9,14H,1-5H3
InchiKey: NNSNIMZGXLISCO-UHFFFAOYSA-N
Formula: C13H20O
SMILES: Cc1cc(O)c(C(C)C)cc1C(C)C
Mol. weight [g/mol]: 192.30
CAS: 40625-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-7.77	kJ/mol	Joback Method
hf	-285.93	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.947		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1496.20		NIST Webbook
rinpol	1496.20		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
ripol	2282.00		NIST Webbook
tb	613.22	K	Joback Method
tc	831.48	K	Joback Method
tf	369.45	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.72	J/mol×K	613.22	Joback Method
cpg	470.84	J/mol×K	649.60	Joback Method
cpg	486.03	J/mol×K	685.97	Joback Method

cpg	500.35	J/mol×K	722.35	Joback Method
cpg	513.88	J/mol×K	758.72	Joback Method
cpg	526.69	J/mol×K	795.10	Joback Method
cpg	538.86	J/mol×K	831.48	Joback Method
dvisc	0.0019088	Pa×s	369.45	Joback Method
dvisc	0.0006436	Pa×s	410.08	Joback Method
dvisc	0.0002640	Pa×s	450.71	Joback Method
dvisc	0.0001255	Pa×s	491.34	Joback Method
dvisc	0.0000668	Pa×s	531.96	Joback Method
dvisc	0.0000389	Pa×s	572.59	Joback Method
dvisc	0.0000243	Pa×s	613.22	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40625965&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume