Phenol, 2,4-bis(1-methylethyl)-

Other names: Phenol, 2,4-diisopropyl-
2,4-Diisopropylphenol
Inchi: InChI=1S/C12H18O/c1-8(2)10-5-6-12(13)11(7-10)9(3)4/h5-9,13H,1-4H3
InchiKey: KEUMBYCOWGLRBQ-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(C)c1ccc(O)c(C(C)C)c1
Mol. weight [g/mol]: 178.27
CAS: 2934-05-6

Physical Properties

Property code	Value	Unit	Source
chl	-6979.00	kJ/mol	NIST Webbook
gf	-6.56	kJ/mol	Joback Method
hf	-254.10 ± 2.80	kJ/mol	NIST Webbook
hf	-228.00	kJ/mol	NIST Webbook
hfl	-310.00	kJ/mol	NIST Webbook
hfus	19.22	kJ/mol	Joback Method
hvap	86.11	kJ/mol	NIST Webbook
hvap	82.00	kJ/mol	NIST Webbook
log10ws	-3.39		Crippen Method
logp	3.639		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	585.36	K	Joback Method
tc	806.59	K	Joback Method
tf	345.66	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.79	J/mol×K	585.36	Joback Method
cpg	421.56	J/mol×K	622.23	Joback Method
cpg	436.33	J/mol×K	659.10	Joback Method

cpg	450.20	J/mol×K	695.97	Joback Method
cpg	463.24	J/mol×K	732.85	Joback Method
cpg	475.53	J/mol×K	769.72	Joback Method
cpg	487.16	J/mol×K	806.59	Joback Method
dvisc	0.0036943	Pa×s	345.66	Joback Method
dvisc	0.0011103	Pa×s	385.61	Joback Method
dvisc	0.0004182	Pa×s	425.56	Joback Method
dvisc	0.0001862	Pa×s	465.51	Joback Method
dvisc	0.0000943	Pa×s	505.46	Joback Method
dvisc	0.0000527	Pa×s	545.41	Joback Method
dvisc	0.0000319	Pa×s	585.36	Joback Method
hvapt	58.40	kJ/mol	461.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2934056&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume