Phenol, 2,4,6-tris(1-methylethyl)-

Other names: 2,4,6-triisopropylphenol
Inchi: InChI=1S/C15H24O/c1-9(2)12-7-13(10(3)4)15(16)14(8-12)11(5)6/h7-11,16H,1-6H3
InchiKey: HVFKKINZIWVNQG-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)c1cc(C(C)C)c(O)c(C(C)C)c1
Mol. weight [g/mol]: 220.35
CAS: 2934-07-8

Physical Properties

Property code	Value	Unit	Source
chl	-8942.50	kJ/mol	NIST Webbook
gf	6.63	kJ/mol	Joback Method
hf	-333.00 ± 3.10	kJ/mol	NIST Webbook
hf	-290.90	kJ/mol	NIST Webbook
hfl	-390.00	kJ/mol	NIST Webbook
hfus	23.08	kJ/mol	Joback Method
hvap	99.10	kJ/mol	NIST Webbook
hvap	99.20	kJ/mol	NIST Webbook
log10ws	-4.57		Crippen Method
logp	4.762		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1516.00		NIST Webbook
tb	658.54	K	Joback Method
tc	873.68	K	Joback Method
tf	376.99	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.27	J/mol×K	658.54	Joback Method
cpg	636.65	J/mol×K	837.82	Joback Method
cpg	622.64	J/mol×K	801.97	Joback Method

cpg	607.87	J/mol×K	766.11	Joback Method
cpg	592.27	J/mol×K	730.25	Joback Method
cpg	575.76	J/mol×K	694.40	Joback Method
cpg	649.98	J/mol×K	873.68	Joback Method
dvisc	0.0000147	Pa×s	658.54	Joback Method
dvisc	0.0000241	Pa×s	611.62	Joback Method
dvisc	0.0000432	Pa×s	564.69	Joback Method
dvisc	0.0000858	Pa×s	517.76	Joback Method
dvisc	0.0001956	Pa×s	470.84	Joback Method
dvisc	0.0005349	Pa×s	423.92	Joback Method
dvisc	0.0018796	Pa×s	376.99	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2934078&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

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
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