Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-

Other names:	1-Hydroxy-4-ethyl-2,6-di-tert-butylbenzene
	2,6-Bis(1,1-dimethylethyl)-4-ethylphenol
	2,6-Di-tert-butyl-4-ethylphenol
	2,6-di-t-Butyl-4-ethylphenol
	4-Ethyl-2,6-di-tert-butylphenol
	Ionol 2
	NSC 14453
	Nocrac M 17
	Phenol, 2,6-bis-(1.1-dimethylethyl)-4-ethyl
	Phenol, 2,6-di-tert-butyl-4-ethyl-
	Sandant 425
	Yoshinox 250
Inchi:	InChI=1S/C16H26O/c1-8-11-9-12(15(2,3)4)14(17)13(10-11)16(5,6)7/h9-10,17H,8H2,1-7H
InchiKey:	BVUXDWXKPROUDO-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	CCc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	234.38
CAS:	4130-42-1

Physical Properties

Property code	Value	Unit	Source
gf	28.05	kJ/mol	Joback Method
hf	-354.79	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	65.23	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.550		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	676.28	K	Joback Method
tc	898.90	K	Joback Method
tf	438.10	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.67	J/mol×K	676.28	Joback Method
cpg	696.44	J/mol×K	861.80	Joback Method
cpg	682.07	J/mol×K	824.69	Joback Method
cpg	666.94	J/mol×K	787.59	Joback Method
cpg	650.91	J/mol×K	750.49	Joback Method
cpg	633.87	J/mol×K	713.38	Joback Method
cpg	710.19	J/mol×K	898.90	Joback Method
dvisc	0.0000110	Pa×s	676.28	Joback Method
dvisc	0.0000170	Pa×s	636.58	Joback Method
dvisc	0.0000278	Pa×s	596.89	Joback Method
dvisc	0.0000490	Pa×s	557.19	Joback Method
dvisc	0.0000942	Pa×s	517.49	Joback Method
dvisc	0.0002017	Pa×s	477.80	Joback Method
dvisc	0.0004957	Pa×s	438.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34889e+01
Coeff. B	-4.26955e+03
Coeff. C	-9.27020e+01
Temperature range (K), min.	416.12
Temperature range (K), max.	614.81

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=C4130421&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume