Phenol, 2,4,6-tri-tert-butyl-

Other names:	2,4,6-Tri-t-butylphenol
	2,4,6-Tri-tert-butyl-1-hydroxybenzene
	2,4,6-Tri-tert-butylhydroxybenzene
	2,4,6-Tri-tert-butylphenol
	2,4,6-Tris(1,1-dimethylethyl)phenol
	2,4,6-Tris(tert-butyl)phenol
	Alkofen B
	NSC 14459
	P 23
	Phenol, 2,4,6-tris(1,1-dimethylethyl)-
	TM 02
	Voidox
Inchi:	InChI=1S/C18H30O/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11,19H,1
InchiKey:	PFEFOYRSMXVNEL-UHFFFAOYSA-N
Formula:	C18H30O
SMILES:	CC(C)(C)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	262.43
CAS:	732-26-3

Physical Properties

Property code	Value	Unit	Source
chs	-10870.00	kJ/mol	NIST Webbook
gf	47.73	kJ/mol	Joback Method
hf	-369.80	kJ/mol	NIST Webbook
hfs	-498.00	kJ/mol	NIST Webbook
hfus	19.18	kJ/mol	Joback Method
hsub	128.10	kJ/mol	NIST Webbook
hsub	84.20 ± 0.50	kJ/mol	NIST Webbook
hsub	87.50 ± 0.40	kJ/mol	NIST Webbook
hsub	85.60 ± 0.42	kJ/mol	NIST Webbook
hsub	128.20	kJ/mol	NIST Webbook
hvap	68.39	kJ/mol	Joback Method
ie	7.82	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-4.96		Crippen Method
logp	5.285		Crippen Method
mcvol	246.590	ml/mol	McGowan Method

pc	1681.03	kPa	Joback Method
tb	551.20	K	NIST Webbook
tc	945.54	K	Joback Method
tf	404.00 ± 2.50	K	NIST Webbook
tf	405.70 ± 0.20	K	NIST Webbook
tf	402.80 ± 1.00	K	NIST Webbook
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.40	J/mol×K	832.18	Joback Method
cpg	829.17	J/mol×K	945.54	Joback Method
cpg	814.17	J/mol×K	907.75	Joback Method
cpg	798.64	J/mol×K	869.96	Joback Method
cpg	727.73	J/mol×K	718.81	Joback Method
cpg	747.11	J/mol×K	756.60	Joback Method
cpg	765.28	J/mol×K	794.39	Joback Method
dvisc	0.0000275	Pa×s	590.93	Joback Method
dvisc	0.0000091	Pa×s	676.18	Joback Method
dvisc	0.0000058	Pa×s	718.81	Joback Method
dvisc	0.0000153	Pa×s	633.56	Joback Method
dvisc	0.0003079	Pa×s	463.06	Joback Method
dvisc	0.0001201	Pa×s	505.69	Joback Method
dvisc	0.0000543	Pa×s	548.31	Joback Method
hfust	19.46	kJ/mol	405.20	NIST Webbook
hfust	19.46	kJ/mol	405.20	NIST Webbook
hsubt	83.90	kJ/mol	302.50	NIST Webbook
hsubt	85.60 ± 0.40	kJ/mol	317.00	NIST Webbook
hvapt	63.20	kJ/mol	483.00	NIST Webbook
sfust	21.66	J/mol×K	405.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28968e+01

Coeff. B	-4.11754e+03
Coeff. C	-9.43700e+01
Temperature range (K), min.	421.15
Temperature range (K), max.	637.15

Sources

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=C732263&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume