6-t-Butyl-2,4-dimethylphenol

Other names:	2,4-Dimethyl-6-tert-butylphenol
	2,4-Xylenol, 6-tert-butyl-
	2-Methyl-6-tert-butyl-p-cresol
	2-tert-Butyl-4,6-dimethylphenol
	6-t-Butyl-2,4-xylenol
	6-tert-Butyl-2,4-xylenol
	NSC 8130
	Phenol, 2-(1,1-dimethylethyl)-4,6-dimethyl-
	Prodox 340
	Topanol A
Inchi:	InChI=1S/C12H18O/c1-8-6-9(2)11(13)10(7-8)12(3,4)5/h6-7,13H,1-5H3
InchiKey:	OPLCSTZDXXUYDU-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	Cc1cc(C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	178.28
CAS:	1879-09-0

Physical Properties

Property code	Value	Unit	Source
hf	-240.07	kJ/mol	Cheméo Relay (1.0)
hfus	18.47	kJ/mol	Joback Method
hvap	68.40 ± 0.80	kJ/mol	NIST Webbook
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-3.49		Cheméo Relay (1.0)
logp	3.307		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1363.90		NIST Webbook
tb	518.53	K	Cheméo Relay (1.0)
tf	327.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.95	J/mol×K	587.99	Joback Method

cpg	487.78	J/mol×K	814.25	Joback Method
cpg	476.42	J/mol×K	776.54	Joback Method
cpg	464.42	J/mol×K	738.83	Joback Method
cpg	451.67	J/mol×K	701.12	Joback Method
cpg	438.08	J/mol×K	663.41	Joback Method
cpg	423.54	J/mol×K	625.70	Joback Method
dvisc	0.0000479	Pa×s	555.09	Joback Method
dvisc	0.0000316	Pa×s	587.99	Joback Method
dvisc	0.0004821	Pa×s	423.50	Joback Method
dvisc	0.0002389	Pa×s	456.40	Joback Method
dvisc	0.0001301	Pa×s	489.30	Joback Method
dvisc	0.0000765	Pa×s	522.19	Joback Method
dvisc	0.0010949	Pa×s	390.60	Joback Method
hvapt	51.70	kJ/mol	439.50	NIST Webbook
hvapt	67.20 ± 0.80	kJ/mol	318.50	NIST Webbook
hvapt	45.40	kJ/mol	439.50	NIST Webbook
hvapt	49.70	kJ/mol	439.50	NIST Webbook
hvapt	58.40	kJ/mol	455.00	NIST Webbook
hvapt	52.70	kJ/mol	439.50	NIST Webbook
hvapt	54.40	kJ/mol	439.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66619e+01
Coeff. B	-5.09917e+03
Coeff. C	-8.63080e+01
Temperature range (K), min.	397.72
Temperature range (K), max.	535.56

Sources

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1879090&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point