4-tert-butyl-2,6-dimethylphenol

Inchi: InChI=1S/C12H18O/c1-8-6-10(12(3,4)5)7-9(2)11(8)13/h6-7,13H,1-5H3
InchiKey: MEPYMUOZRROULQ-UHFFFAOYSA-N
Formula: C12H18O
SMILES: Cc1cc(C(C)(C)C)cc(C)c1O
Mol. weight [g/mol]: 178.28
CAS: 879-97-0

Physical Properties

Property code	Value	Unit	Source
hf	-251.08	kJ/mol	Cheméo Relay (1.0)
hfus	18.47	kJ/mol	Joback Method
hvap	79.57	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-3.40		Cheméo Relay (1.0)
logp	3.307		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	511.11	K	Cheméo Relay (1.0)
tc	745.49	K	Cheméo Relay (1.0)
tf	365.17	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	0.0001301	Pa×s	489.30	Joback Method
dvisc	0.0000316	Pa×s	587.99	Joback Method
dvisc	0.0000479	Pa×s	555.09	Joback Method

dvisc	0.0000765	Pa×s	522.19	Joback Method
dvisc	0.0010949	Pa×s	390.60	Joback Method
dvisc	0.0002389	Pa×s	456.40	Joback Method
dvisc	0.0004821	Pa×s	423.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54518e+01
Coeff. B	-4.71440e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	396.92
Temperature range (K), max.	550.95

Sources

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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