4-t-Butyl-o-xylene

Other names:	1,2-Dimethyl-4-tert-butylbenzene
	1-tert-Butyl-3,4-dimethylbenzene
	3,4-Dimethyl-tert-butylbenzene
	4-tert-Butyl-1,2-dimethylbenzene
	4-tert-Butyl-o-xylene
	Benzene, 1,2-dimethyl-4-(1,1-dimethylethyl)
	Benzene, 1,2-dimethyl-4-tert-butyl
	Benzene, 4-(1,1-dimethylethyl)-1,2-dimethyl-
	o-Xylene, 4-tert-butyl-
Inchi:	InChI=1S/C12H18/c1-9-6-7-11(8-10(9)2)12(3,4)5/h6-8H,1-5H3
InchiKey:	QRPPSTNABSMSCS-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	Cc1ccc(C(C)(C)C)cc1C
Mol. weight [g/mol]:	162.27
CAS:	7397-06-0

Physical Properties

Property code	Value	Unit	Source
gf	146.15	kJ/mol	Joback Method
hf	-86.17	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.601		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1205.00		NIST Webbook
rinpol	1192.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	507.37	K	Joback Method
tc	722.03	K	Joback Method
tf	278.88	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.74	J/mol×K	507.37	Joback Method
cpg	367.17	J/mol×K	543.15	Joback Method
cpg	383.55	J/mol×K	578.92	Joback Method
cpg	398.95	J/mol×K	614.70	Joback Method
cpg	413.40	J/mol×K	650.48	Joback Method
cpg	426.96	J/mol×K	686.25	Joback Method
cpg	439.68	J/mol×K	722.03	Joback Method
dvisc	0.0025008	Pa×s	278.88	Joback Method
dvisc	0.0012488	Pa×s	316.96	Joback Method
dvisc	0.0007238	Pa×s	355.04	Joback Method
dvisc	0.0004663	Pa×s	393.12	Joback Method
dvisc	0.0003246	Pa×s	431.21	Joback Method
dvisc	0.0002397	Pa×s	469.29	Joback Method
dvisc	0.0001852	Pa×s	507.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.00 ± 1.00	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47344e+01
Coeff. B	-4.08763e+03
Coeff. C	-7.40760e+01
Temperature range (K), min.	357.02
Temperature range (K), max.	507.87

Sources

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
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=C7397060&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume