Naphthalene, 1-(1,1-dimethylethyl)-

Other names:	1-(1,1-Dimethylethyl)naphthalene
	1-tert-Butylnaphthalene
	Naphthalene, 1-tert-butyl-
	«alpha»-tert-Butylnaphthalene
	Â«alphaÂ»-tert-Butylnaphthalene
Inchi:	InChI=1S/C14H16/c1-14(2,3)13-10-6-8-11-7-4-5-9-12(11)13/h4-10H,1-3H3
InchiKey:	SPLGZANLVHBDCC-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	CC(C)(C)c1cccc2ccccc12
Mol. weight [g/mol]:	184.28
CAS:	17085-91-5

Physical Properties

Property code	Value	Unit	Source
gf	279.27	kJ/mol	Joback Method
hf	75.09	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	50.04	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.137		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	551.00 ± 6.00	K	NIST Webbook
tb	561.00 ± 5.00	K	NIST Webbook
tb	552.00 ± 4.00	K	NIST Webbook
tc	803.55	K	Joback Method
tf	321.60	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	393.23	J/mol×K	567.13	Joback Method
cpg	410.99	J/mol×K	606.53	Joback Method
cpg	427.37	J/mol×K	645.94	Joback Method
cpg	442.47	J/mol×K	685.34	Joback Method
cpg	456.40	J/mol×K	724.74	Joback Method
cpg	469.28	J/mol×K	764.14	Joback Method
cpg	481.23	J/mol×K	803.55	Joback Method
dvisc	0.0020663	Pa×s	321.60	Joback Method
dvisc	0.0011977	Pa×s	362.52	Joback Method
dvisc	0.0007754	Pa×s	403.44	Joback Method
dvisc	0.0005439	Pa×s	444.37	Joback Method
dvisc	0.0004050	Pa×s	485.29	Joback Method
dvisc	0.0003157	Pa×s	526.21	Joback Method
dvisc	0.0002551	Pa×s	567.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44311e+01
Coeff. B	-4.64199e+03
Coeff. C	-7.89430e+01
Temperature range (K), min.	407.15
Temperature range (K), max.	587.96

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=C17085915&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