Naphthalene, 2-(1,1-dimethylethyl)-

Other names:	2-(1,1-Dimethylethyl)naphthalene 2-tert-Butylnaphthalene Naphthalene, 2-tert-butyl- «beta»-tert-Butylnaphthalene Â«betaÂ»-tert-Butylnaphthalene
Inchi:	InChI=1S/C14H16/c1-14(2,3)13-9-8-11-6-4-5-7-12(11)10-13/h4-10H,1-3H3
InchiKey:	MCEORGGPAKTORV-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	CC(C)(C)c1ccc2ccccc2c1
Mol. weight [g/mol]:	184.28
CAS:	2876-35-9

Physical Properties

Property code	Value	Unit	Source
chl	-7769.50 ± 1.30	kJ/mol	NIST Webbook
gf	279.27	kJ/mol	Joback Method
hf	75.09	kJ/mol	Joback Method
hfl	-26.30 ± 1.50	kJ/mol	NIST Webbook
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	1475.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	549.00 ± 6.00	K	NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tb	554.80 ± 4.00	K	NIST Webbook
tb	558.00 ± 15.00	K	NIST Webbook
tb	550.00 ± 5.00	K	NIST Webbook
tc	803.55	K	Joback Method
tf	267.00 ± 4.00	K	NIST Webbook
tf	354.00 ± 4.00	K	NIST Webbook
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	469.28	J/mol×K	764.14	Joback Method
cpg	456.40	J/mol×K	724.74	Joback Method
cpg	442.47	J/mol×K	685.34	Joback Method
cpg	427.37	J/mol×K	645.94	Joback Method
cpg	410.99	J/mol×K	606.53	Joback Method
cpg	481.23	J/mol×K	803.55	Joback Method
dvisc	0.0002551	Pa×s	567.13	Joback Method
dvisc	0.0003157	Pa×s	526.21	Joback Method
dvisc	0.0004050	Pa×s	485.29	Joback Method
dvisc	0.0005439	Pa×s	444.37	Joback Method
dvisc	0.0007754	Pa×s	403.44	Joback Method
dvisc	0.0011977	Pa×s	362.52	Joback Method
dvisc	0.0020663	Pa×s	321.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44790e+01
Coeff. B	-4.77092e+03
Coeff. C	-7.09660e+01
Temperature range (K), min.	407.15
Temperature range (K), max.	591.38

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=C2876359&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

chl:	Standard liquid 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
hfl:	Liquid phase 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

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