Naphthalene, 1-(1-methylethyl)-

Other names:	1-Isopropylnaphthalene
	Naphthalene, 1-isopropyl-
	«alpha»-Isopropylnaphthalene
	Â«alphaÂ»-Isopropylnaphthalene
Inchi:	InChI=1S/C13H14/c1-10(2)12-9-5-7-11-6-3-4-8-13(11)12/h3-10H,1-2H3
InchiKey:	PMPBFICDXLLSRM-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	CC(C)c1cccc2ccccc12
Mol. weight [g/mol]:	170.25
CAS:	6158-45-8

Physical Properties

Property code	Value	Unit	Source
gf	265.57	kJ/mol	Joback Method
hf	99.20	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.963		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1451.10		NIST Webbook
rinpol	1465.90		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1460.90		NIST Webbook
rinpol	1451.10		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1465.90		NIST Webbook
rinpol	1460.90		NIST Webbook
tb	547.04	K	Joback Method
tc	778.34	K	Joback Method
tf	257.49 ± 0.10	K	NIST Webbook
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.66	J/mol×K	547.04	Joback Method
cpg	359.12	J/mol×K	585.59	Joback Method
cpg	374.41	J/mol×K	624.14	Joback Method
cpg	388.61	J/mol×K	662.69	Joback Method
cpg	401.80	J/mol×K	701.24	Joback Method
cpg	414.06	J/mol×K	739.79	Joback Method
cpg	425.45	J/mol×K	778.34	Joback Method
dvisc	0.0020244	Pa×s	292.91	Joback Method
dvisc	0.0011772	Pa×s	335.26	Joback Method
dvisc	0.0007731	Pa×s	377.62	Joback Method
dvisc	0.0005526	Pa×s	419.98	Joback Method
dvisc	0.0004201	Pa×s	462.33	Joback Method
dvisc	0.0003344	Pa×s	504.68	Joback Method
dvisc	0.0002758	Pa×s	547.04	Joback Method
hvapt	50.40	kJ/mol	471.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45036e+01
Coeff. B	-4.37353e+03
Coeff. C	-9.65700e+01
Temperature range (K), min.	404.22
Temperature range (K), max.	572.36

Sources

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=C6158458&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume