Naphthalene, 1,7-dimethyl-

Other names: 1,7-Dimethylnaphthalene
Naphthalene, 3,5-dimethyl
Inchi: InChI=1S/C12H12/c1-9-6-7-11-5-3-4-10(2)12(11)8-9/h3-8H,1-2H3
InchiKey: SPUWFVKLHHEKGV-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc2cccc(C)c2c1
Mol. weight [g/mol]: 156.22
CAS: 575-37-1

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	243.20		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1418.70		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1409.50		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	242.99		NIST Webbook
rinpol	240.66		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	243.75		NIST Webbook
rinpol	243.05		NIST Webbook
rinpol	242.19		NIST Webbook
rinpol	242.90		NIST Webbook
rinpol	242.77		NIST Webbook

rinpol	240.66		NIST Webbook
rinpol	243.80		NIST Webbook
rinpol	1422.40		NIST Webbook
rinpol	244.29		NIST Webbook
rinpol	242.60		NIST Webbook
rinpol	244.10		NIST Webbook
rinpol	242.80		NIST Webbook
rinpol	242.80		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1389.60		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	240.70		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	531.00 ± 4.00	K	NIST Webbook
tb	536.20	K	KDB
tb	535.00 ± 4.00	K	NIST Webbook
tb	536.00 ± 4.00	K	NIST Webbook
tb	535.90 ± 2.00	K	NIST Webbook
tb	536.00 ± 1.00	K	NIST Webbook
tc	770.60	K	KDB
tf	260.00	K	KDB
vc	0.521	m3/kmol	KDB
zc	0.2449940		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.31	J/mol×K	529.58	Joback Method
cpg	361.06	J/mol×K	722.55	Joback Method
cpg	349.89	J/mol×K	683.95	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cpg	371.48	J/mol×K	761.14	Joback Method

dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40634e+01
Coeff. B	-3.94601e+03
Coeff. C	-1.18215e+02
Temperature range (K), min.	404.66
Temperature range (K), max.	569.09

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol775.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C575371&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
zc:	Critical Compressibility