Naphthalene, 2,7-dimethyl-

Other names: 2,7-Dimethylnaphthalene
Inchi: InChI=1S/C12H12/c1-9-3-5-11-6-4-10(2)8-12(11)7-9/h3-8H,1-2H3
InchiKey: LRQYSMQNJLZKPS-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc2ccc(C)cc2c1
Mol. weight [g/mol]: 156.22
CAS: 582-16-1

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
chs	-6431.69 ± 0.96	kJ/mol	NIST Webbook
gf	249.96	kJ/mol	Joback Method
hf	79.50 ± 0.60	kJ/mol	NIST Webbook
hfs	-5.40 ± 1.10	kJ/mol	NIST Webbook
hfus	22.20	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hvap	47.55	kJ/mol	Joback Method
ie	7.89 ± 0.03	eV	NIST Webbook
log10ws	-4.23		Crippen Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3234.00 ± 100.00	kPa	NIST Webbook
pc	3200.00 ± 200.00	kPa	NIST Webbook
pc	3230.00	kPa	KDB
rhoc	265.58 ± 31.24	kg/m3	NIST Webbook
rhoc	254.64 ± 29.68	kg/m3	NIST Webbook
rinpol	1409.50		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1392.10		NIST Webbook
rinpol	1402.20		NIST Webbook
rinpol	1409.50		NIST Webbook
rinpol	1392.10		NIST Webbook

rinpol	1402.20		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.20		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1390.10		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	240.99		NIST Webbook
rinpol	237.71		NIST Webbook
rinpol	240.56		NIST Webbook
rinpol	240.04		NIST Webbook
rinpol	240.50		NIST Webbook
rinpol	240.28		NIST Webbook
rinpol	237.71		NIST Webbook
rinpol	240.30		NIST Webbook
rinpol	237.70		NIST Webbook
rinpol	241.13		NIST Webbook
rinpol	240.30		NIST Webbook
rinpol	240.50		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.20		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1409.50		NIST Webbook
rinpol	1390.10		NIST Webbook
rinpol	1380.40		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1392.10		NIST Webbook
sl	283.36	J/mol×K	NIST Webbook
ss	228.57	J/mol×K	NIST Webbook
tb	538.00 ± 4.00	K	NIST Webbook
tb	536.20	K	KDB
tb	536.20	K	NIST Webbook
tc	775.00	K	KDB
tc	775.00 ± 2.00	K	NIST Webbook
tc	775.00 ± 2.00	K	NIST Webbook
tf	370.15 ± 0.50	K	NIST Webbook
tf	369.10	K	Solid-Liquid Phase Equilibria of Binary and Ternary Mixtures for 2,6-Dimethylnaphthalene and 2,7-Dimethylnaphthalene with Ethanol or Methanol
tf	371.00	K	KDB
tt	368.81 ± 0.03	K	NIST Webbook
tt	368.81 ± 0.02	K	NIST Webbook
vc	0.601	m3/kmol	KDB

vc	0.601	m3/kmol	NIST Webbook
zc	0.3012580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.48	J/mol×K	761.14	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	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
cpl	251.85	J/mol×K	298.15	NIST Webbook
cps	204.39	J/mol×K	298.15	NIST Webbook
cps	202.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
hfust	22.20	kJ/mol	370.20	NIST Webbook
hfust	23.35	kJ/mol	368.80	NIST Webbook
hfust	23.35	kJ/mol	368.80	NIST Webbook
hfust	23.35	kJ/mol	368.81	NIST Webbook
hsubt	84.60	kJ/mol	350.50	NIST Webbook
hsubt	84.00 ± 1.00	kJ/mol	354.50	NIST Webbook
hsubt	83.20	kJ/mol	369.00	NIST Webbook
hvapt	49.50	kJ/mol	520.00	NIST Webbook
hvapt	58.10	kJ/mol	383.50	NIST Webbook
hvapt	58.60	kJ/mol	383.50	NIST Webbook
hvapt	59.50	kJ/mol	383.50	NIST Webbook
hvapt	58.50	kJ/mol	384.50	NIST Webbook
hvapt	46.60	kJ/mol	560.00	NIST Webbook
hvapt	52.20	kJ/mol	480.00	NIST Webbook
hvapt	54.80	kJ/mol	440.00	NIST Webbook
hvapt	57.30	kJ/mol	400.00	NIST Webbook
sfust	63.32	J/mol×K	368.81	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40520e+01
Coeff. B	-3.97246e+03
Coeff. C	-1.15106e+02
Temperature range (K), min.	370.15
Temperature range (K), max.	569.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.67212e+01
Coeff. B	-8.91493e+03
Coeff. C	-5.70208e+00
Coeff. D	1.22633e-06
Temperature range (K), min.	368.81
Temperature range (K), max.	778.00

Sources

Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=778
KDB:	https://www.cheric.org/files/research/kdb/mol/mol778.mol
Solid-Liquid Phase Equilibria of Binary and Ternary Mixtures for 2,6-Dimethylnaphthalene and 2,7-Dimethylnaphthalene with Ethanol or Methanol:	https://www.doi.org/10.1021/je049607b
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C582161&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

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility