1,8-Dimethylnaphthalene

Inchi: InChI=1S/C12H12/c1-9-5-3-7-11-8-4-6-10(2)12(9)11/h3-8H,1-2H3
InchiKey: XAABPYINPXYOLM-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1cccc2cccc(C)c12
Mol. weight [g/mol]: 156.23
CAS: 569-41-5

Physical Properties

Property code	Value	Unit	Source
af	0.4178		Cheméo Relay (1.0)
chs	-6463.00 ± 1.00	kJ/mol	NIST Webbook
chs	-6463.20 ± 2.60	kJ/mol	NIST Webbook
gf	249.96	kJ/mol	Joback Method
hf	108.60	kJ/mol	NIST Webbook
hf	108.80 ± 3.00	kJ/mol	NIST Webbook
hfs	26.10 ± 3.00	kJ/mol	NIST Webbook
hfs	25.90 ± 1.20	kJ/mol	NIST Webbook
hfus	18.53	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hsub	82.70 ± 0.30	kJ/mol	NIST Webbook
hsub	82.70	kJ/mol	NIST Webbook
hsub	82.70 ± 0.30	kJ/mol	NIST Webbook
hvap	64.87	kJ/mol	Cheméo Relay (1.0)
ie	7.64 ± 0.03	eV	NIST Webbook
ie	7.71	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-4.15		Cheméo Relay (1.0)
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1472.40		NIST Webbook
rinpol	1472.10		NIST Webbook
rinpol	249.39		NIST Webbook
rinpol	250.70		NIST Webbook
rinpol	1472.70		NIST Webbook

rinpol	1459.70		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1440.80		NIST Webbook
rinpol	1456.80		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1472.70		NIST Webbook
rinpol	1472.10		NIST Webbook
rinpol	1459.70		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1459.70		NIST Webbook
rinpol	1472.70		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1440.80		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	249.39		NIST Webbook
rinpol	252.00		NIST Webbook
rinpol	249.52		NIST Webbook
rinpol	250.70		NIST Webbook
rinpol	249.52		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1989.00		NIST Webbook
ss	224.72	J/mol×K	NIST Webbook
tb	526.12	K	Cheméo Relay (1.0)
tc	773.22	K	Cheméo Relay (1.0)
tf	335.00 ± 2.00	K	NIST Webbook
tt	336.32 ± 0.02	K	NIST Webbook
tt	336.32 ± 0.02	K	NIST Webbook
tt	336.32 ± 0.02	K	NIST Webbook
vc	0.505	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	296.31	J/mol×K	529.58	Joback Method
cpg	371.48	J/mol×K	761.14	Joback Method
cps	242.80	J/mol×K	298.15	NIST Webbook
cps	241.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
hfust	0.05	kJ/mol	336.33	NIST Webbook
hfust	15.77	kJ/mol	336.30	NIST Webbook
hfust	0.05	kJ/mol	336.33	NIST Webbook
hfust	18.53	kJ/mol	338.20	NIST Webbook
hfust	15.77	kJ/mol	336.30	NIST Webbook
hsubt	77.90	kJ/mol	332.00	NIST Webbook
hsubt	79.60	kJ/mol	336.00	NIST Webbook
hvapt	60.70	kJ/mol	375.50	NIST Webbook
hvapt	62.20	kJ/mol	375.50	NIST Webbook
hvapt	60.70	kJ/mol	375.50	NIST Webbook
hvapt	59.70	kJ/mol	375.50	NIST Webbook
hvapt	64.80	kJ/mol	375.50	NIST Webbook
hvapt	59.70	kJ/mol	375.50	NIST Webbook
hvapt	62.20	kJ/mol	375.50	NIST Webbook
hvapt	64.80	kJ/mol	375.50	NIST Webbook
hvapt	62.80	kJ/mol	375.50	NIST Webbook
sfust	46.86	J/mol×K	336.33	NIST Webbook
sfust	46.86	J/mol×K	336.33	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58900e+01
Coeff. B	-4.93899e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	402.00
Temperature range (K), max.	552.34

Sources

New aspects of relationship between the enthalpies of fusion of aromatic compounds at the melting temperatures and the enthalpies of solution in benzene at 298.15 K. Part I:	https://www.doi.org/10.1016/j.jct.2017.09.006
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C569415&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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

hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume