Naphthalene, 1,6,7-trimethyl-

Other names: 1,6,7-Trimethylnaphthalene
2,3,5-Trimethylnaphthalene
Naphthalene, 2,3,5-trimethyl-
Inchi: InChI=1S/C13H14/c1-9-5-4-6-12-7-10(2)11(3)8-13(9)12/h4-8H,1-3H3
InchiKey: JBXULKRNHAQMAS-UHFFFAOYSA-N
Formula: C13H14
SMILES: Cc1cc2cccc(C)c2cc1C
Mol. weight [g/mol]: 170.25
CAS: 2245-38-7

Physical Properties

Property code	Value	Unit	Source
gf	248.75	kJ/mol	Joback Method
hf	81.54	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.765		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	266.94		NIST Webbook
rinpol	267.94		NIST Webbook
rinpol	266.94		NIST Webbook
rinpol	269.34		NIST Webbook
rinpol	267.12		NIST Webbook
rinpol	267.50		NIST Webbook
rinpol	1552.00		NIST Webbook

rinpol	267.61		NIST Webbook
rinpol	267.43		NIST Webbook
rinpol	265.81		NIST Webbook
rinpol	267.54		NIST Webbook
rinpol	265.90		NIST Webbook
rinpol	266.50		NIST Webbook
rinpol	265.90		NIST Webbook
rinpol	265.90		NIST Webbook
rinpol	265.90		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	266.50		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	267.50		NIST Webbook
rinpol	267.54		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	265.58		NIST Webbook
rinpol	266.94		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	557.44	K	Joback Method
tc	785.77	K	Joback Method
tf	298.65 ± 0.50	K	NIST Webbook
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/mol×K	557.44	Joback Method
cpg	357.34	J/mol×K	595.49	Joback Method
cpg	371.70	J/mol×K	633.55	Joback Method
cpg	385.15	J/mol×K	671.60	Joback Method
cpg	397.73	J/mol×K	709.66	Joback Method
cpg	409.52	J/mol×K	747.71	Joback Method
cpg	420.56	J/mol×K	785.77	Joback Method
dvisc	0.0010939	Pa×s	332.95	Joback Method
dvisc	0.0007795	Pa×s	370.37	Joback Method
dvisc	0.0005911	Pa×s	407.78	Joback Method
dvisc	0.0004696	Pa×s	445.20	Joback Method
dvisc	0.0003866	Pa×s	482.61	Joback Method
dvisc	0.0003273	Pa×s	520.03	Joback Method

dvisc	0.0002834	Pa×s	557.44	Joback Method
hvapt	68.60	kJ/mol	398.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	558.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55003e+01
Coeff. B	-5.04223e+03
Coeff. C	-7.97010e+01
Temperature range (K), min.	411.15
Temperature range (K), max.	574.58

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2245387&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

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

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
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