

Naphthalene, 2,3,6-trimethyl-

Other names:	2,3,6-Trimethylnaphthalene
Inchi:	InChI=1S/C13H14/c1-9-4-5-12-7-10(2)11(3)8-13(12)6-9/h4-8H,1-3H3
InchiKey:	UNBZRJCHIWTUHB-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	Cc1ccc2cc(C)c(C)cc2c1
Mol. weight [g/mol]:	170.25
CAS:	829-26-5

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	1515.00		NIST Webbook
rinpol	1544.10		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1509.73		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	264.76		NIST Webbook
rinpol	264.98		NIST Webbook
rinpol	263.83		NIST Webbook
rinpol	265.30		NIST Webbook
rinpol	261.83		NIST Webbook
rinpol	265.43		NIST Webbook
rinpol	265.16		NIST Webbook
rinpol	1529.40		NIST Webbook

rinpol	263.20		NIST Webbook
rinpol	264.66		NIST Webbook
rinpol	264.99		NIST Webbook
rinpol	263.87		NIST Webbook
rinpol	263.25		NIST Webbook
rinpol	265.09		NIST Webbook
rinpol	263.31		NIST Webbook
rinpol	264.99		NIST Webbook
rinpol	263.31		NIST Webbook
rinpol	264.60		NIST Webbook
rinpol	265.00		NIST Webbook
rinpol	265.10		NIST Webbook
rinpol	263.31		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	265.43		NIST Webbook
rinpol	264.99		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	265.10		NIST Webbook
rinpol	264.76		NIST Webbook
tb	536.70	K	NIST Webbook
tb	537.00 ± 5.00	K	NIST Webbook
tc	785.77	K	Joback Method
tf	370.00 ± 0.60	K	NIST Webbook
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/molxK	557.44	Joback Method
cpg	357.34	J/molxK	595.49	Joback Method
cpg	371.70	J/molxK	633.55	Joback Method
cpg	385.15	J/molxK	671.60	Joback Method
cpg	397.73	J/molxK	709.66	Joback Method
cpg	409.52	J/molxK	747.71	Joback Method
cpg	420.56	J/molxK	785.77	Joback Method
dvisc	0.0010939	Paxs	332.95	Joback Method
dvisc	0.0007795	Paxs	370.37	Joback Method
dvisc	0.0005911	Paxs	407.78	Joback Method
dvisc	0.0004696	Paxs	445.20	Joback Method

dvisc	0.0003866	Paxs	482.61	Joback Method
dvisc	0.0003273	Paxs	520.03	Joback Method
dvisc	0.0002834	Paxs	557.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54961e+01
Coeff. B	-4.75783e+03
Coeff. C	-9.93100e+01
Temperature range (K), min.	412.15
Temperature range (K), max.	566.47

Sources

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C829265&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	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

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