Naphthalene, 1,2,3-trimethyl-

Other names:	1,2,3-trimethylnaphthalene
	Naphthalene, 2,3,4-trimethyl
Inchi:	InChI=1S/C13H14/c1-9-8-12-6-4-5-7-13(12)11(3)10(9)2/h4-8H,1-3H3
InchiKey:	RQHPYGROUIBUSW-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	Cc1cc2ccccc2c(C)c1C
Mol. weight [g/mol]:	170.25
CAS:	879-12-9

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	1590.00		NIST Webbook
rinpol	264.56		NIST Webbook
rinpol	263.31		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	557.44	K	Joback Method
tc	785.77	K	Joback Method
tf	301.60 ± 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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42860e+01
Coeff. B	-3.49700e+03
Coeff. C	-1.81335e+02
Temperature range (K), min.	431.15
Temperature range (K), max.	571.00

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C879129&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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