Naphthalene, 2,3,4-trimethyl

Other names: 1,2,3-trimethylnaphthalene
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]: 170.26
CAS: 879-12-9

Physical Properties

Property code	Value	Unit	Source
af	0.4430		Cheméo Relay (1.0)
gf	248.75	kJ/mol	Joback Method
hf	90.40	kJ/mol	Cheméo Relay (1.0)
hfus	19.32	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Cheméo Relay (1.0)
ie	7.57	eV	Cheméo Relay (1.0)
log10ws	-4.92		Cheméo Relay (1.0)
logp	3.765		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	263.31		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	264.56		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	557.78	K	Cheméo Relay (1.0)
tc	797.86	K	Cheméo Relay (1.0)
tf	301.60 ± 0.50	K	NIST Webbook
vc	0.563	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/mol×K	557.44	Joback Method
cpg	420.56	J/mol×K	785.77	Joback Method

cpg	409.52	J/mol×K	747.71	Joback Method
cpg	397.73	J/mol×K	709.66	Joback Method
cpg	385.15	J/mol×K	671.60	Joback Method
cpg	371.70	J/mol×K	633.55	Joback Method
cpg	357.34	J/mol×K	595.49	Joback Method
dvisc	0.0004696	Pa×s	445.20	Joback Method
dvisc	0.0002834	Pa×s	557.44	Joback Method
dvisc	0.0003273	Pa×s	520.03	Joback Method
dvisc	0.0003866	Pa×s	482.61	Joback Method
dvisc	0.0010939	Pa×s	332.95	Joback Method
dvisc	0.0005911	Pa×s	407.78	Joback Method
dvisc	0.0007795	Pa×s	370.37	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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C879129&Units=SI

Legend

af:	Acentric Factor
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume