Naphthalene, 1,2,5-trimethyl-

Other names: 1,2,5-Trimethylnaphthalene
Inchi: InChI=1S/C13H14/c1-9-7-8-12-10(2)5-4-6-13(12)11(9)3/h4-8H,1-3H3
InchiKey: KTDQNLIDLMRHCJ-UHFFFAOYSA-N
Formula: C13H14
SMILES: Cc1ccc2c(C)cccc2c1C
Mol. weight [g/mol]: 170.25
CAS: 641-91-8

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	269.47		NIST Webbook
rinpol	270.00		NIST Webbook
rinpol	270.52		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	270.75		NIST Webbook
rinpol	269.50		NIST Webbook
tb	557.44	K	Joback Method
tc	785.77	K	Joback Method
tf	332.95	K	Joback Method
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	1.55935e+01
Coeff. B	-5.15536e+03
Coeff. C	-7.33280e+01
Temperature range (K), min.	410.15
Temperature range (K), max.	574.72

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C641918&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
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