

1,4,6,7-Tetramethylnaphthalene

Inchi:	InChI=1S/C14H16/c1-9-5-6-10(2)14-8-12(4)11(3)7-13(9)14/h5-8H,1-4H3
InchiKey:	VPSPONBLZCLIU-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	Cc1cc2c(C)ccc(C)c2cc1C
Mol. weight [g/mol]:	184.28
CAS:	13764-18-6

Physical Properties

Property code	Value	Unit	Source
gf	247.54	kJ/mol	Joback Method
hf	49.43	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.073		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	287.18		NIST Webbook
rinpol	287.18		NIST Webbook
tb	585.30	K	Joback Method
tc	810.38	K	Joback Method
tf	356.74	K	Joback Method
vc	0.633	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.23	J/mol×K	585.30	Joback Method
cpg	405.02	J/mol×K	622.81	Joback Method
cpg	419.87	J/mol×K	660.33	Joback Method
cpg	433.83	J/mol×K	697.84	Joback Method
cpg	446.95	J/mol×K	735.36	Joback Method
cpg	459.28	J/mol×K	772.87	Joback Method
cpg	470.88	J/mol×K	810.38	Joback Method

dvisc	0.0009613	Paxs	356.74	Joback Method
dvisc	0.0007025	Paxs	394.83	Joback Method
dvisc	0.0005425	Paxs	432.93	Joback Method
dvisc	0.0004369	Paxs	471.02	Joback Method
dvisc	0.0003634	Paxs	509.11	Joback Method
dvisc	0.0003101	Paxs	547.21	Joback Method
dvisc	0.0002702	Paxs	585.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63870e+01
Coeff. B	-5.38420e+03
Coeff. C	-1.03895e+02
Temperature range (K), min.	438.33
Temperature range (K), max.	590.03

Sources

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=R576444&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/ci9903071

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
mccvol:	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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