1,4,5,8-TETRAMETHYLNAPHTHALENE

Inchi: InChI=1S/C14H16/c1-9-5-6-11(3)14-12(4)8-7-10(2)13(9)14/h5-8H,1-4H3
InchiKey: DWUSGRRPJCRNCI-UHFFFAOYSA-N
Formula: C14H16
SMILES: Cc1ccc(C)c2c(C)ccc(C)c12
Mol. weight [g/mol]: 184.28
CAS: 2717-39-7

Physical Properties

Property code	Value	Unit	Source
af	0.5104		Cheméo Relay (1.0)
chs	-7777.60 ± 2.80	kJ/mol	NIST Webbook
gf	247.54	kJ/mol	Joback Method
hf	81.60 ± 3.60	kJ/mol	NIST Webbook
hfs	-18.20 ± 3.40	kJ/mol	NIST Webbook
hfus	21.52	kJ/mol	Joback Method
hsub	99.80 ± 1.40	kJ/mol	NIST Webbook
hsub	99.80	kJ/mol	NIST Webbook
hsub	99.80 ± 1.40	kJ/mol	NIST Webbook
hvap	74.03	kJ/mol	Cheméo Relay (1.0)
ie	7.58	eV	Cheméo Relay (1.0)
log10ws	-5.19		Cheméo Relay (1.0)
logp	4.073		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
tb	559.07	K	Cheméo Relay (1.0)
tc	796.03	K	Cheméo Relay (1.0)
tf	404.00 ± 4.00	K	NIST Webbook
vc	0.617	m3/kmol	Cheméo Relay (1.0)

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	Pa×s	356.74	Joback Method
dvisc	0.0007025	Pa×s	394.83	Joback Method
dvisc	0.0005425	Pa×s	432.93	Joback Method
dvisc	0.0004369	Pa×s	471.02	Joback Method
dvisc	0.0003634	Pa×s	509.11	Joback Method
dvisc	0.0003101	Pa×s	547.21	Joback Method
dvisc	0.0002702	Pa×s	585.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

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=C2717397&Units=SI

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):

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume