

Naphthalene, 1,2,3,4-tetrahydro-1,5-dimethyl-

Other names:	1,2,3,4-Tetrahydro-1,5-dimethylnaphthalene 1,5-Dimethyltetralin 1,5-Dimethyltetraline
Inchi:	InChI=1S/C12H16/c1-9-5-3-8-12-10(2)6-4-7-11(9)12/h3,5,8,10H,4,6-7H2,1-2H3
InchiKey:	BMADLDGHUBLVMQ-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	Cc1cccc2c1CCCC2C
Mol. weight [g/mol]:	160.26
CAS:	21564-91-0

Physical Properties

Property code	Value	Unit	Source
gf	191.96	kJ/mol	Joback Method
hf	-10.78	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.435		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpola	229.85		NIST Webbook
tb	521.61	K	Joback Method
tc	747.23	K	Joback Method
tf	290.88	K	Joback Method
vc	0.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.07	J/molxK	521.61	Joback Method
cpg	351.33	J/molxK	559.21	Joback Method
cpg	368.45	J/molxK	596.82	Joback Method
cpg	384.49	J/molxK	634.42	Joback Method
cpg	399.49	J/molxK	672.02	Joback Method

cpg	413.53	J/molxK	709.63	Joback Method
cpg	426.65	J/molxK	747.23	Joback Method
dvisc	0.0016585	Paxs	290.88	Joback Method
dvisc	0.0010799	Paxs	329.33	Joback Method
dvisc	0.0007692	Paxs	367.79	Joback Method
dvisc	0.0005842	Paxs	406.25	Joback Method
dvisc	0.0004653	Paxs	444.70	Joback Method
dvisc	0.0003843	Paxs	483.16	Joback Method
dvisc	0.0003265	Paxs	521.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35870e+01
Coeff. B	-3.90859e+03
Coeff. C	-8.35280e+01
Temperature range (K), min.	377.42
Temperature range (K), max.	555.84

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=C21564910&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
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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