NAPHTHALENE, 1-PROPYL-

Other names:	1-Propylnaphthalene
	1-n-Propylnaphthalene
Inchi:	InChI=1S/C13H14/c1-2-6-11-8-5-9-12-7-3-4-10-13(11)12/h3-5,7-10H,2,6H2,1H3
InchiKey:	HMAMGXMFMCAOPV-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	CCCc1cccc2ccccc12
Mol. weight [g/mol]:	170.26
CAS:	27378-74-1

Physical Properties

Property code	Value	Unit	Source
af	0.4578		Cheméo Relay (1.0)
gf	268.01	kJ/mol	Joback Method
hf	83.49	kJ/mol	Cheméo Relay (1.0)
hfus	20.10	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Cheméo Relay (1.0)
ie	7.90	eV	Cheméo Relay (1.0)
log10ws	-4.84		Cheméo Relay (1.0)
logp	3.792		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	545.92	K	Cheméo Relay (1.0)
tc	774.76	K	Cheméo Relay (1.0)
tf	267.20	K	Cheméo Relay (1.0)
vc	0.571	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.33	J/mol×K	547.48	Joback Method
cpg	358.36	J/mol×K	585.17	Joback Method
cpg	373.27	J/mol×K	622.85	Joback Method
cpg	387.16	J/mol×K	660.54	Joback Method
cpg	400.09	J/mol×K	698.22	Joback Method

cpg	412.12	J/mol×K	735.91	Joback Method
cpg	423.35	J/mol×K	773.60	Joback Method
dvisc	0.0016610	Pa×s	307.91	Joback Method
dvisc	0.0010543	Pa×s	347.84	Joback Method
dvisc	0.0007349	Pa×s	387.77	Joback Method
dvisc	0.0005480	Pa×s	427.70	Joback Method
dvisc	0.0004296	Pa×s	467.62	Joback Method
dvisc	0.0003499	Pa×s	507.55	Joback Method
dvisc	0.0002937	Pa×s	547.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49034e+01
Coeff. B	-4.90449e+03
Coeff. C	-6.91470e+01
Temperature range (K), min.	404.71
Temperature range (K), max.	580.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.16094e+02
Coeff. B	-1.23594e+04
Coeff. C	-1.43577e+01
Coeff. D	5.56389e-06
Temperature range (K), min.	428.15
Temperature range (K), max.	771.45

Sources

Cheméo Relay (1.0, beta):

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=782

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2765186&Units=SI
Cheméo Relay (1.0):	

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