

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:	HMAMGXMFMAOPV-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	CCc1cccc2cccc12
Mol. weight [g/mol]:	170.25
CAS:	2765-18-6

Physical Properties

Property code	Value	Unit	Source
chl	-6820.00	kJ/mol	NIST Webbook
gf	268.01	kJ/mol	Joback Method
hf	104.48	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	49.11	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.792		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	255.10		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	547.48	K	Joback Method
tc	773.60	K	Joback Method
tf	365.00 ± 2.00	K	NIST Webbook
tf	264.55 ± 0.20	K	NIST Webbook
vc	0.578	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.33	J/molxK	547.48	Joback Method
cpg	358.36	J/molxK	585.17	Joback Method
cpg	373.27	J/molxK	622.85	Joback Method
cpg	387.16	J/molxK	660.54	Joback Method
cpg	400.09	J/molxK	698.22	Joback Method
cpg	412.12	J/molxK	735.91	Joback Method
cpg	423.35	J/molxK	773.60	Joback Method
dvisc	0.0016610	Paxs	307.91	Joback Method
dvisc	0.0010543	Paxs	347.84	Joback Method
dvisc	0.0007349	Paxs	387.77	Joback Method
dvisc	0.0005480	Paxs	427.69	Joback Method
dvisc	0.0004296	Paxs	467.62	Joback Method
dvisc	0.0003499	Paxs	507.55	Joback Method
dvisc	0.0002937	Paxs	547.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2765186&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=782

Legend

chl:	Standard liquid 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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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