1-Pentylnaphthalene

Inchi: InChI=1S/C15H18/c1-2-3-4-8-13-10-7-11-14-9-5-6-12-15(13)14/h5-7,9-12H,2-4,8H2,1H3
InchiKey: FDHDUXOBMHHFFJ-UHFFFAOYSA-N
Formula: C15H18
SMILES: CCCCCc1cccc2ccccc12
Mol. weight [g/mol]: 198.30
CAS: 1320-27-0

Physical Properties

Property code	Value	Unit	Source
af	0.5750		KDB
chl	-8033.00	kJ/mol	NIST Webbook
gf	284.85	kJ/mol	Joback Method
hf	63.20	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.572		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2270.00	kPa	KDB
tb	580.20	K	KDB
tc	793.30	K	KDB
tf	251.00	K	KDB
vc	0.690	m3/kmol	KDB
zc	0.2372940		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.22	J/mol×K	593.24	Joback Method
cpg	456.44	J/mol×K	629.58	Joback Method
cpg	472.55	J/mol×K	665.92	Joback Method
cpg	487.61	J/mol×K	702.25	Joback Method
cpg	501.70	J/mol×K	738.59	Joback Method
cpg	514.89	J/mol×K	774.93	Joback Method

cpg	527.24	J/mol×K	811.27	Joback Method
dvisc	0.0017537	Pa×s	330.45	Joback Method
dvisc	0.0010653	Pa×s	374.25	Joback Method
dvisc	0.0007184	Pa×s	418.05	Joback Method
dvisc	0.0005221	Pa×s	461.85	Joback Method
dvisc	0.0004009	Pa×s	505.64	Joback Method
dvisc	0.0003212	Pa×s	549.44	Joback Method
dvisc	0.0002658	Pa×s	593.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53740e+01
Coeff. B	-5.59367e+03
Coeff. C	-5.69350e+01
Temperature range (K), min.	427.71
Temperature range (K), max.	612.82

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.37042e+02
Coeff. B	-1.43160e+04
Coeff. C	-1.72754e+01
Coeff. D	6.48132e-06
Temperature range (K), min.	458.15
Temperature range (K), max.	793.32

Sources

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=797
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

KDB:	https://www.cheric.org/files/research/kdb/mol/mol797.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1320270&Units=SI

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility