

Indane, 1-phenyl

Inchi:	InChI=1S/C15H14/c1-2-6-12(7-3-1)15-11-10-13-8-4-5-9-14(13)15/h1-9,15H,10-11H2
InchiKey:	VNAFWALXWOAPCK-UHFFFAOYSA-N
Formula:	C15H14
SMILES:	<chem>c1ccc(C2CCc3ccccc32)cc1</chem>
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	351.36	kJ/mol	Joback Method
hf	181.46	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.765		Crippen Method
mcvol	163.830	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rmpol	1618.00		NIST Webbook
tb	607.68	K	Joback Method
tc	861.33	K	Joback Method
tf	342.11	K	Joback Method
vc	0.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.94	J/molxK	607.68	Joback Method
cpg	425.64	J/molxK	649.95	Joback Method
cpg	442.78	J/molxK	692.23	Joback Method
cpg	458.49	J/molxK	734.50	Joback Method
cpg	472.90	J/molxK	776.78	Joback Method
cpg	486.15	J/molxK	819.05	Joback Method
cpg	498.37	J/molxK	861.33	Joback Method
dvisc	0.0018621	Paxs	342.11	Joback Method
dvisc	0.0012365	Paxs	386.37	Joback Method

dvisc	0.0008932	Paxs	430.63	Joback Method
dvisc	0.0006855	Paxs	474.89	Joback Method
dvisc	0.0005504	Paxs	519.16	Joback Method
dvisc	0.0004575	Paxs	563.42	Joback Method
dvisc	0.0003906	Paxs	607.68	Joback Method

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=R73004&Units=SI

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
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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