Phthalan

Other names: 1,3-Dihydro isobenzofuran
Isobenzofuran, 1,3-dihydro-
Isobenzofuran
Inchi: InChI=1S/C8H8O/c1-2-4-8-6-9-5-7(8)3-1/h1-4H,5-6H2
InchiKey: SFLGSKRGOWRGBR-UHFFFAOYSA-N
Formula: C8H8O
SMILES: c1ccc2c(c1)COC2
Mol. weight [g/mol]: 120.15
CAS: 496-14-0

Physical Properties

Property code	Value	Unit	Source
chl	-4207.57 ± 0.54	kJ/mol	NIST Webbook
gf	101.60	kJ/mol	Joback Method
hf	-30.10 ± 1.00	kJ/mol	NIST Webbook
hfl	-83.83 ± 0.93	kJ/mol	NIST Webbook
hfus	15.17	kJ/mol	Joback Method
hvap	53.74 ± 0.42	kJ/mol	NIST Webbook
hvap	53.70 ± 0.40	kJ/mol	NIST Webbook
hvap	53.70	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	1.717		Crippen Method
mcvol	94.830	ml/mol	McGowan Method
pc	4285.00 ± 400.00	kPa	NIST Webbook
rhoc	337.26 ± 20.43	kg/m3	NIST Webbook
tb	465.20	K	NIST Webbook
tc	700.00 ± 4.00	K	NIST Webbook
tf	267.61	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.41	J/mol×K	452.46	Joback Method

cpg	200.19	J/mol×K	490.67	Joback Method
cpg	211.99	J/mol×K	528.88	Joback Method
cpg	222.87	J/mol×K	567.10	Joback Method
cpg	232.90	J/mol×K	605.31	Joback Method
cpg	242.14	J/mol×K	643.52	Joback Method
cpg	250.67	J/mol×K	681.73	Joback Method
cpl	188.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0020452	Pa×s	267.61	Joback Method
dvisc	0.0013881	Pa×s	298.42	Joback Method
dvisc	0.0010130	Pa×s	329.23	Joback Method
dvisc	0.0007802	Pa×s	360.04	Joback Method
dvisc	0.0006262	Pa×s	390.84	Joback Method
dvisc	0.0005189	Pa×s	421.65	Joback Method
dvisc	0.0004412	Pa×s	452.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C496140&Units=SI
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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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

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