Naphthalene, 1-(phenylmethyl)-

Other names: 1-Benzylnaphthalene
Inchi: InChI=1S/C17H14/c1-2-7-14(8-3-1)13-16-11-6-10-15-9-4-5-12-17(15)16/h1-12H,13H2
InchiKey: KTHUKEZOIFYPEH-UHFFFAOYSA-N
Formula: C17H14
SMILES: c1ccc(Cc2cccc3ccccc23)cc1
Mol. weight [g/mol]: 218.29
CAS: 611-45-0

Physical Properties

Property code	Value	Unit	Source
gf	414.10	kJ/mol	Joback Method
hf	258.45	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	60.29	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.431		Crippen Method
mcvol	183.410	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	332.88		NIST Webbook
tb	665.68	K	Joback Method
tc	922.07	K	Joback Method
tf	331.00 ± 4.00	K	NIST Webbook
tf	331.00	K	NIST Webbook
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.17	J/mol×K	665.68	Joback Method
cpg	535.63	J/mol×K	879.34	Joback Method
cpg	523.50	J/mol×K	836.61	Joback Method
cpg	510.32	J/mol×K	793.87	Joback Method
cpg	495.97	J/mol×K	751.14	Joback Method
cpg	480.30	J/mol×K	708.41	Joback Method

cpg	546.87	J/mol×K	922.07	Joback Method
dvisc	0.0002379	Pa×s	665.68	Joback Method
dvisc	0.0002874	Pa×s	617.97	Joback Method
dvisc	0.0003583	Pa×s	570.26	Joback Method
dvisc	0.0004651	Pa×s	522.55	Joback Method
dvisc	0.0006361	Pa×s	474.83	Joback Method
dvisc	0.0009333	Pa×s	427.12	Joback Method
dvisc	0.0015077	Pa×s	379.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.70	K	2.50	NIST Webbook
tbrp	491.50 ± 1.50	K	2.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611450&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume