Benzene, 1-methyl-2-(phenylmethyl)-

Other names:	1-Methyl-2-benzylbenzene
	2'-Methyldiphenylmethane
	2-Benzyltoluene
	2-Methyldiphenylmethane
	Methane, phenyl-o-tolyl-
	NSC 75366
	Phenyl-2-tolylmethane
	Phenyl-o-tolylmethane
	o-Benzyltoluene
	o-Tolylphenylmethane
	«alpha»-Phenyl-o-xylene
	Â«alphaÂ»-Phenyl-o-xylene
Inchi:	InChI=1S/C14H14/c1-12-7-5-6-10-14(12)11-13-8-3-2-4-9-13/h2-10H,11H2,1H3
InchiKey:	PQTAUFTUHHRKSS-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1ccccc1Cc1ccccc1
Mol. weight [g/mol]:	182.26
CAS:	713-36-0

Physical Properties

Property code	Value	Unit	Source
chl	-7259.00	kJ/mol	NIST Webbook
gf	282.19	kJ/mol	Joback Method
hf	129.30	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.586		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1570.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2179.00		NIST Webbook
sl	335.50	J/mol×K	NIST Webbook
tb	553.65 ± 0.50	K	NIST Webbook
tb	553.65 ± 0.40	K	NIST Webbook

tc	818.72	K	Joback Method
tf	279.76 ± 0.05	K	NIST Webbook
tt	279.76 ± 0.01	K	NIST Webbook
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.94	J/mol×K	818.72	Joback Method
cpg	447.19	J/mol×K	778.61	Joback Method
cpg	434.45	J/mol×K	738.50	Joback Method
cpg	420.65	J/mol×K	698.39	Joback Method
cpg	405.71	J/mol×K	658.28	Joback Method
cpg	389.56	J/mol×K	618.17	Joback Method
cpg	372.14	J/mol×K	578.06	Joback Method
cpl	296.58	J/mol×K	298.15	NIST Webbook
dvisc	0.0006118	Pa×s	401.29	Joback Method
dvisc	0.0001748	Pa×s	578.06	Joback Method
dvisc	0.0019467	Pa×s	312.90	Joback Method
dvisc	0.0002212	Pa×s	533.87	Joback Method
dvisc	0.0002920	Pa×s	489.67	Joback Method
dvisc	0.0004075	Pa×s	445.48	Joback Method
dvisc	0.0010159	Pa×s	357.09	Joback Method
hfust	19.24	kJ/mol	279.76	NIST Webbook
hfust	19.24	kJ/mol	279.80	NIST Webbook
sfust	68.78	J/mol×K	279.76	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45704e+01
Coeff. B	-4.63970e+03
Coeff. C	-8.74450e+01
Temperature range (K), min.	412.29
Temperature range (K), max.	588.55

Sources

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=C713360&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume