Benzene, (1-methylheptyl)-

Other names: (1-Methylheptyl)benzene
2-Phenyloctane
Octane, 2-phenyl-
Inchi: InChI=1S/C14H22/c1-3-4-5-7-10-13(2)14-11-8-6-9-12-14/h6,8-9,11-13H,3-5,7,10H2,1-2H
InchiKey: GTYIGAUPHJCMLF-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCCCC(C)c1ccccc1
Mol. weight [g/mol]: 190.32
CAS: 777-22-0

Physical Properties

Property code	Value	Unit	Source
gf	176.97	kJ/mol	Joback Method
hf	-101.04	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	70.00	kJ/mol	NIST Webbook
log10ws	-4.75		Crippen Method
logp	4.761		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1358.00		NIST Webbook
tb	522.65 ± 0.50	K	NIST Webbook
tc	744.01	K	Joback Method
tf	234.30 ± 0.50	K	NIST Webbook
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.50	J/mol×K	744.01	Joback Method
cpg	442.13	J/mol×K	545.96	Joback Method
cpg	460.73	J/mol×K	578.97	Joback Method
cpg	478.33	J/mol×K	611.98	Joback Method
cpg	494.96	J/mol×K	644.99	Joback Method
cpg	510.68	J/mol×K	678.00	Joback Method
cpg	525.51	J/mol×K	711.00	Joback Method
dvisc	0.0001693	Pa×s	545.96	Joback Method
dvisc	0.0053384	Pa×s	258.96	Joback Method
dvisc	0.0019183	Pa×s	306.79	Joback Method
dvisc	0.0009085	Pa×s	354.63	Joback Method
dvisc	0.0005139	Pa×s	402.46	Joback Method
dvisc	0.0003281	Pa×s	450.29	Joback Method
dvisc	0.0002284	Pa×s	498.13	Joback Method
hvapt	61.60	kJ/mol	376.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38447e+01
Coeff. B	-4.12602e+03
Coeff. C	-8.68040e+01
Temperature range (K), min.	391.15
Temperature range (K), max.	570.33

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=C777220&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume