

Benzene, (1-methylbutyl)-

Other names:	(1-Methybutyl)benzene
	(1-Methylbutyl)benzene
	(dl) 2-phenylpentane
	1-Methyl-1-Phenylbutane
	1-Methyl-n-butylbenzene
	1-Phenyl-1-methylbutane
	2-Phenylpentane
	Benzene, sec-pentyl- sec-Pentylbenzene
Inchi:	InChI=1S/C11H16/c1-3-7-10(2)11-8-5-4-6-9-11/h4-6,8-10H,3,7H2,1-2H3
InchiKey:	LTHAIAJHDPJXLG-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCC(C)c1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	2719-52-0

Physical Properties

Property code	Value	Unit	Source
gf	151.71	kJ/mol	Joback Method
hf	-39.12	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.590		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1078.10		NIST Webbook
rinpol	1082.10		NIST Webbook
rinpol	1071.59		NIST Webbook

rinpol	1078.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1077.80		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1074.70		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1324.30		NIST Webbook
ripol	1324.30		NIST Webbook
tb	477.32	K	Joback Method
tc	683.92	K	Joback Method
tf	225.15	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.07	J/mol×K	477.32	Joback Method
cpg	316.59	J/mol×K	511.75	Joback Method
cpg	332.19	J/mol×K	546.19	Joback Method
cpg	346.91	J/mol×K	580.62	Joback Method
cpg	360.78	J/mol×K	615.05	Joback Method
cpg	373.84	J/mol×K	649.49	Joback Method
cpg	386.13	J/mol×K	683.92	Joback Method
dvisc	0.0057730	Pa×s	225.15	Joback Method
dvisc	0.0021444	Pa×s	267.18	Joback Method
dvisc	0.0010427	Pa×s	309.21	Joback Method
dvisc	0.0006024	Pa×s	351.24	Joback Method
dvisc	0.0003914	Pa×s	393.26	Joback Method
dvisc	0.0002764	Pa×s	435.29	Joback Method
dvisc	0.0002075	Pa×s	477.32	Joback Method
hvapt	50.30	kJ/mol	384.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.43026e+01
Coeff. B	-3.80497e+03
Coeff. C	-7.02500e+01
Temperature range (K), min.	341.74
Temperature range (K), max.	493.44

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2719520&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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