

Benzene, 1-methyl-2-pentyl

Other names:	1-methyl-2-n-pentylbenzene
Inchi:	InChI=1S/C12H18/c1-3-4-5-9-12-10-7-6-8-11(12)/h6-8,10H,3-5,9H2,1-2H3
InchiKey:	NQVHSBDSEAYZOO-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCCCc1ccccc1C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	152.94	kJ/mol	Joback Method
hf	-65.95	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.728		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1236.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1238.50		NIST Webbook
rinpol	1242.30		NIST Webbook
rinpol	1247.10		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1238.50		NIST Webbook
rinpol	1249.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1489.20		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1539.00		NIST Webbook

ripol	1555.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1489.00		NIST Webbook
tb	505.62	K	Joback Method
tc	706.05	K	Joback Method
tf	263.94	K	Joback Method
vc	0.600	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.19	J/molxK	505.62	Joback Method
cpg	420.54	J/molxK	672.64	Joback Method
cpg	407.24	J/molxK	639.24	Joback Method
cpg	393.19	J/molxK	605.83	Joback Method
cpg	378.35	J/molxK	572.43	Joback Method
cpg	362.69	J/molxK	539.02	Joback Method
cpg	433.10	J/molxK	706.05	Joback Method
dvisc	0.0002000	Paxs	505.62	Joback Method
dvisc	0.0002551	Paxs	465.34	Joback Method
dvisc	0.0003409	Paxs	425.06	Joback Method
dvisc	0.0004839	Paxs	384.78	Joback Method
dvisc	0.0007455	Paxs	344.50	Joback Method
dvisc	0.0012879	Paxs	304.22	Joback Method
dvisc	0.0026290	Paxs	263.94	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R13599&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

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

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