

Benzene, 1-methyl-3-pentyl

Other names:	1-Methyl-3-n-Pentylbenzene
Inchi:	InChI=1S/C12H18/c1-3-4-5-8-12-9-6-7-11(2)10-12/h6-7,9-10H,3-5,8H2,1-2H3
InchiKey:	LULWNWYYCJANEM-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCCCc1cccc(C)c1
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	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
ripol	1464.70		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	505.62	K	Joback Method
tc	706.05	K	Joback Method
tf	263.94	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=R52818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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