Pentane, 1-methoxy-

Other names:	1-METHOXYPENTANE
	Amyl methyl ether
	Ether, methyl pentyl
	METHYL PENTYL ETHER
	Methyl amyl ether
	N-AMYL METHYL ETHER
	Pentyl methyl ether
	n-C5H11OCH3
Inchi:	InChI=1S/C6H14O/c1-3-4-5-6-7-2/h3-6H2,1-2H3
InchiKey:	DBUJFULDVAZULB-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCCCCOC
Mol. weight [g/mol]:	102.17
CAS:	628-80-8

Physical Properties

Property code	Value	Unit	Source
af	0.3470		KDB
gf	-105.36	kJ/mol	Joback Method
hf	-299.39	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	36.91	kJ/mol	NIST Webbook
ie	9.67	eV	NIST Webbook
log10ws	-1.42		Crippen Method
logp	1.823		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3042.00 ± 50.66	kPa	NIST Webbook
pc	3042.00	kPa	KDB
rhoc	268.72 ± 4.09	kg/m3	NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	722.10		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	722.10		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	705.00		NIST Webbook
ripol	774.00		NIST Webbook

ripol	774.00		NIST Webbook
tb	372.70	K	NIST Webbook
tb	372.00	K	KDB
tb	372.00	K	NIST Webbook
tc	546.53 ± 1.00	K	NIST Webbook
tc	546.49 ± 2.00	K	NIST Webbook
tc	546.53	K	KDB
tf	179.61	K	Joback Method
vc	0.392 ± 0.003	m3/kmol	NIST Webbook
vc	0.391	m3/kmol	KDB
zc	0.2617490		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.55	J/mol×K	523.60	Joback Method
cpg	181.85	J/mol×K	359.10	Joback Method
cpg	191.99	J/mol×K	386.52	Joback Method
cpg	201.86	J/mol×K	413.93	Joback Method
cpg	211.45	J/mol×K	441.35	Joback Method
cpg	220.76	J/mol×K	468.76	Joback Method
cpg	229.79	J/mol×K	496.18	Joback Method
dvisc	0.0002210	Pa×s	359.10	Joback Method
dvisc	0.0035470	Pa×s	179.61	Joback Method
dvisc	0.0016051	Pa×s	209.53	Joback Method
dvisc	0.0008855	Pa×s	239.44	Joback Method
dvisc	0.0005575	Pa×s	269.36	Joback Method
dvisc	0.0003850	Pa×s	299.27	Joback Method
dvisc	0.0002844	Pa×s	329.19	Joback Method
hvapt	32.02	kJ/mol	372.00	NIST Webbook
rhol	750.00	kg/m3	298.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53730e+01

Coeff. B	-3.52145e+03
Coeff. C	-4.45660e+01
Temperature range (K), min.	278.00
Temperature range (K), max.	394.56

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1013.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628808&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
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

zc: Critical Compressibility