Benzaldehyde, 4-methyl-

Other names:	4-Methylbenzaldehyde
	4-Tolualdehyde
	NSC 2224
	P-FORMYLTOLUENE
	P-METHYLBENZALDEHYDE
	P-TOLUALDEHYDE
	P-TOLYLALDEHYDE
	PTAL
	Paratolualdehyde
	p-Toluylaldehyde
Inchi:	InChI=1S/C8H8O/c1-7-2-4-8(6-9)5-3-7/h2-6H,1H3
InchiKey:	FXLOVSHXALFLKQ-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	Cc1ccc(C=O)cc1
Mol. weight [g/mol]:	120.15
CAS:	104-87-0

Physical Properties

Property code	Value	Unit	Source
affp	851.80	kJ/mol	NIST Webbook
basg	820.00	kJ/mol	NIST Webbook
ea	0.37 ± 0.02	eV	NIST Webbook
gf	19.74	kJ/mol	Joback Method
hf	-68.97	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
ie	9.33 ± 0.05	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.808		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1081.00		NIST Webbook

rinpol	1074.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	174.20		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1073.90		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1073.90		NIST Webbook
rinpol	1083.60		NIST Webbook
rinpol	1074.60		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1076.10		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1079.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1605.00		NIST Webbook
tb	477.70	K	NIST Webbook

tc	712.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	260.86	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.28	J/mol×K	462.76	Joback Method
cpg	242.88	J/mol×K	643.76	Joback Method
cpg	234.35	J/mol×K	607.56	Joback Method
cpg	225.25	J/mol×K	571.36	Joback Method
cpg	215.55	J/mol×K	535.16	Joback Method
cpg	205.24	J/mol×K	498.96	Joback Method
cpg	250.87	J/mol×K	679.96	Joback Method
dvisc	0.0002879	Pa×s	462.76	Joback Method
dvisc	0.0003551	Pa×s	429.11	Joback Method
dvisc	0.0004540	Pa×s	395.46	Joback Method
dvisc	0.0006075	Pa×s	361.81	Joback Method
dvisc	0.0008630	Pa×s	328.16	Joback Method
dvisc	0.0013282	Pa×s	294.51	Joback Method
dvisc	0.0022848	Pa×s	260.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47996e+01
Coeff. B	-4.16349e+03
Coeff. C	-6.87640e+01
Temperature range (K), min.	355.66
Temperature range (K), max.	507.57

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.69627e+01
Coeff. B	-9.73128e+03
Coeff. C	-1.01911e+01
Coeff. D	3.91264e-06
Temperature range (K), min.	289.85
Temperature range (K), max.	698.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1248
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1248
Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method:	https://www.doi.org/10.1016/j.fluid.2014.07.038
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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
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