Benzaldehyde, 2-methyl-

Other names:	2-Formyltoluene
	2-Methylbenzaldehyde
	2-Tolualdehyde
	NSC 103152
	o-Methylbenzaldehyde
	o-Tolualdehyde
	o-Toluic aldehyde
	o-Toluylaldehyde
	o-Tolylaldehyde
Inchi:	InChI=1S/C8H8O/c1-7-4-2-3-5-8(7)6-9/h2-6H,1H3
InchiKey:	BTFQKIATRPGRBS-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	Cc1ccccc1C=O
Mol. weight [g/mol]:	120.15
CAS:	529-20-4

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-2.19		Crippen Method
logp	1.808		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1034.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1065.60		NIST Webbook
rinpol	1070.90		NIST Webbook

rinpol	1067.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1054.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1621.00		NIST Webbook
tb	467.15 ± 3.00	K	NIST Webbook
tb	473.20	K	NIST Webbook
tc	679.96	K	Joback 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	205.24	J/mol×K	498.96	Joback Method
cpg	215.55	J/mol×K	535.16	Joback Method
cpg	225.25	J/mol×K	571.36	Joback Method
cpg	234.35	J/mol×K	607.56	Joback Method
cpg	242.88	J/mol×K	643.76	Joback Method
cpg	250.87	J/mol×K	679.96	Joback Method
dvisc	0.0022848	Pa×s	260.86	Joback Method
dvisc	0.0013282	Pa×s	294.51	Joback Method
dvisc	0.0008630	Pa×s	328.16	Joback Method
dvisc	0.0006075	Pa×s	361.81	Joback Method
dvisc	0.0004540	Pa×s	395.46	Joback Method
dvisc	0.0003551	Pa×s	429.11	Joback Method
dvisc	0.0002879	Pa×s	462.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51175e+01
Coeff. B	-4.20214e+03
Coeff. C	-7.29640e+01
Temperature range (K), min.	356.32
Temperature range (K), max.	501.49

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=C529204&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

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
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