Benzaldehyde, 3-methyl-

Other names:	m-Tolualdehyde
	m-Methylbenzaldehyde
	3-Methylbenzaldehyde
	m-Toluylaldehyde
	3-CH3C6H4CHO
Inchi:	InChI=1S/C8H8O/c1-7-3-2-4-8(5-7)6-9/h2-6H,1H3
InchiKey:	OVWYEQOVUDKZNU-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	Cc1cccc(C=O)c1
Mol. weight [g/mol]:	120.15
CAS:	620-23-5

Physical Properties

Property code	Value	Unit	Source
affp	840.00	kJ/mol	NIST Webbook
basg	808.10	kJ/mol	NIST Webbook
ea	0.41 ± 0.01	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
log10ws	-2.19		Crippen Method
logp	1.808		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1070.40		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1060.60		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook

ripol	1628.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	472.20	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	2.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620235&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume