Benzaldehyde, 2,4-dimethyl-

Other names:	2,4-Dimethylbenzaldehyde
	2,4-Dimethylbenzenecarboxaldehyde
Inchi:	InChI=1S/C9H10O/c1-7-3-4-9(6-10)8(2)5-7/h3-6H,1-2H3
InchiKey:	GISVICWQYMUPJF-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	Cc1ccc(C=O)c(C)c1
Mol. weight [g/mol]:	134.18
CAS:	15764-16-6

Physical Properties

Property code	Value	Unit	Source
gf	18.53	kJ/mol	Joback Method
hf	-101.08	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.116		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1143.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1710.00		NIST Webbook
tb	490.62	K	Joback Method
tc	705.85	K	Joback Method
tf	284.65	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.09	J/mol×K	490.62	Joback Method
cpg	246.84	J/mol×K	526.49	Joback Method
cpg	257.95	J/mol×K	562.36	Joback Method
cpg	268.44	J/mol×K	598.24	Joback Method
cpg	278.35	J/mol×K	634.11	Joback Method
cpg	287.67	J/mol×K	669.98	Joback Method
cpg	296.44	J/mol×K	705.85	Joback Method
dvisc	0.0017961	Pa×s	284.65	Joback Method
dvisc	0.0011064	Pa×s	318.98	Joback Method
dvisc	0.0007489	Pa×s	353.31	Joback Method
dvisc	0.0005432	Pa×s	387.63	Joback Method
dvisc	0.0004151	Pa×s	421.96	Joback Method
dvisc	0.0003303	Pa×s	456.29	Joback Method
dvisc	0.0002714	Pa×s	490.62	Joback Method
hvapt	57.40	kJ/mol	423.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.00	K	1.90	NIST Webbook
tbrp	372.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68754e+01
Coeff. B	-5.58943e+03
Coeff. C	-3.51350e+01
Temperature range (K), min.	372.09

Temperature range (K), max.	518.48

Sources

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=C15764166&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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