Benzaldehyde, 2,5-dimethyl-

Other names:	Isoxylaldehyde
	2,5-Dimethylbenzaldehyde
Inchi:	InChI=1S/C9H10O/c1-7-3-4-8(2)9(5-7)6-10/h3-6H,1-2H3
InchiKey:	SMUVABOERCFKRW-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	Cc1ccc(C)c(C=O)c1
Mol. weight [g/mol]:	134.18
CAS:	5779-94-2

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	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1154.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1680.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	1.90	NIST Webbook

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=C5779942&Units=SI

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
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