Benzaldehyde, 2-ethoxy-

Other names:	Benzaldehyde, o-ethoxy-
	o-Ethoxybenzaldehyde
	2-Ethoxybenzaldehyde
	ortho-Ethoxybenzaldehyde
Inchi:	InChI=1S/C9H10O2/c1-2-11-9-6-4-3-5-8(9)7-10/h3-7H,2H2,1H3
InchiKey:	DUVJMSPTZMCSTQ-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CCOc1ccccc1C=O
Mol. weight [g/mol]:	150.17
CAS:	613-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-76.84	kJ/mol	Joback Method
hf	-221.83	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	47.70	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.898		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1286.40		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
tb	521.20	K	NIST Webbook
tc	719.99	K	Joback Method
tf	294.36	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.62	J/mol×K	508.06	Joback Method
cpg	310.99	J/mol×K	684.67	Joback Method

cpg	301.51	J/mol×K	649.35	Joback Method
cpg	291.44	J/mol×K	614.02	Joback Method
cpg	280.78	J/mol×K	578.70	Joback Method
cpg	269.51	J/mol×K	543.38	Joback Method
cpg	319.90	J/mol×K	719.99	Joback Method
dvisc	0.0002417	Pa×s	508.06	Joback Method
dvisc	0.0002999	Pa×s	472.44	Joback Method
dvisc	0.0003855	Pa×s	436.83	Joback Method
dvisc	0.0005181	Pa×s	401.21	Joback Method
dvisc	0.0007377	Pa×s	365.59	Joback Method
dvisc	0.0011334	Pa×s	329.98	Joback Method
dvisc	0.0019322	Pa×s	294.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	3.20	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C613694&Units=SI

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