Benzaldehyde, 3-ethyl-

Other names:	3-Ethylbenzaldehyde
	m-ethylbenzaldehyde
Inchi:	InChI=1S/C9H10O/c1-2-8-4-3-5-9(6-8)7-10/h3-7H,2H2,1H3
InchiKey:	LLYXUFQXCNIGDG-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CCc1cccc(C=O)c1
Mol. weight [g/mol]:	134.18
CAS:	34246-54-3

Physical Properties

Property code	Value	Unit	Source
gf	28.16	kJ/mol	Joback Method
hf	-89.61	kJ/mol	Joback Method
hfus	15.01	kJ/mol	Joback Method
hvap	45.29	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.062		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	1168.00		NIST Webbook
tb	485.64	K	Joback Method
tc	699.60	K	Joback Method
tf	272.13	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.04	J/mol×K	485.64	Joback Method
cpg	247.20	J/mol×K	521.30	Joback Method
cpg	258.65	J/mol×K	556.96	Joback Method
cpg	269.43	J/mol×K	592.62	Joback Method
cpg	279.56	J/mol×K	628.28	Joback Method
cpg	289.07	J/mol×K	663.94	Joback Method

cpg	297.98	J/mol×K	699.60	Joback Method
dvisc	0.0024281	Pa×s	272.13	Joback Method
dvisc	0.0013782	Pa×s	307.71	Joback Method
dvisc	0.0008797	Pa×s	343.30	Joback Method
dvisc	0.0006110	Pa×s	378.88	Joback Method
dvisc	0.0004517	Pa×s	414.47	Joback Method
dvisc	0.0003503	Pa×s	450.06	Joback Method
dvisc	0.0002820	Pa×s	485.64	Joback Method

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=C34246543&Units=SI
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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