4-ethylbenzaldehyde

Other names:	ethylbenzaldehyde
	Benzaldehyde, 4-ethyl-
	p-Ethylbenzaldehyde
	4-ethylbenzenecarbaldehyde
	Benzaldehyde, ethyl-
Inchi:	InChI=1S/C9H10O/c1-2-8-3-5-9(7-10)6-4-8/h3-7H,2H2,1H3
InchiKey:	QNGNSVIICDLXHT-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CCc1ccc(C=O)cc1
Mol. weight [g/mol]:	134.18
CAS:	53951-50-1

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	1164.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	197.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1175.00		NIST Webbook

rinpol	1169.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	197.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1731.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53951501&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

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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume