Benzaldehyde, 2-ethyl-

Other names: 2-Ethylbenzaldehyde
Inchi: InChI=1S/C9H10O/c1-2-8-5-3-4-6-9(8)7-10/h3-7H,2H2,1H3
InchiKey: NTWBHJYRDKBGBR-UHFFFAOYSA-N
Formula: C9H10O
SMILES: CCc1ccccc1C=O
Mol. weight [g/mol]: 134.18
CAS: 22927-13-5

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	1176.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1176.00		NIST Webbook
tb	482.20	K	NIST Webbook
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.70	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22927135&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume