Benzeneacetaldehyde, 4-methyl-

Other names: p-Tolyl-acetaldehyde
Inchi: InChI=1S/C9H10O/c1-8-2-4-9(5-3-8)6-7-10/h2-5,7H,6H2,1H3
InchiKey: CIXAYNMKFFQEFU-UHFFFAOYSA-N
Formula: C9H10O
SMILES: Cc1ccc(CC=O)cc1
Mol. weight [g/mol]: 134.18
CAS: 104-09-6

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	-2.03		Crippen Method
logp	1.736		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	1119.90		NIST Webbook
rinpol	1119.90		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1772.00		NIST Webbook
tb	494.70	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	289.07	J/mol×K	663.94	Joback Method
cpg	279.56	J/mol×K	628.28	Joback Method
cpg	269.43	J/mol×K	592.62	Joback Method

cpg	258.65	J/mol×K	556.96	Joback Method
cpg	247.20	J/mol×K	521.30	Joback Method
cpg	297.98	J/mol×K	699.60	Joback Method
dvisc	0.0002820	Pa×s	485.64	Joback Method
dvisc	0.0003503	Pa×s	450.06	Joback Method
dvisc	0.0004517	Pa×s	414.47	Joback Method
dvisc	0.0006110	Pa×s	378.88	Joback Method
dvisc	0.0008797	Pa×s	343.30	Joback Method
dvisc	0.0013782	Pa×s	307.71	Joback Method
dvisc	0.0024281	Pa×s	272.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104096&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume