

Benzeneacetaldehyde

Other names:	.alpha.-tolualdehyde 2-Phenylacetaldehyde 2-phenylethanal Acetaldehyde, phenyl- Benzacetaldehyde Benzenacetaldehyde Benzylcarboxaldehyde Hyacinthin NSC 406309 Phenylacetic aldehyde phenylacetadehyde phenylacetalaldehyde phenylacetaldehyde phenylethanal «alpha»-Tolualdehyde «alpha»-Toluic aldehyde
Inchi:	InChI=1S/C8H8O/c9-7-6-8-4-2-1-3-5-8/h1-5,7H,6H2
InchiKey:	DTUQWGWMMVIHBKE-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	O=CCc1ccccc1
Mol. weight [g/mol]:	120.15
CAS:	122-78-1

Physical Properties

Property code	Value	Unit	Source
gf	29.37	kJ/mol	Joback Method
hf	-57.50	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	54.50	kJ/mol	NIST Webbook
hvap	59.80 ± 0.30	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.30 ± 0.10	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	1.428		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
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tb	468.20	K	NIST Webbook
tc	673.59	K	Joback Method
tf	248.34	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.99	J/mol×K	457.78	Joback Method
cpg	205.42	J/mol×K	493.75	Joback Method
cpg	216.14	J/mol×K	529.72	Joback Method
cpg	226.17	J/mol×K	565.69	Joback Method
cpg	235.55	J/mol×K	601.65	Joback Method
cpg	244.30	J/mol×K	637.62	Joback Method
cpg	252.46	J/mol×K	673.59	Joback Method
dvisc	0.0003808	Pa×s	422.87	Joback Method
dvisc	0.0005010	Pa×s	387.97	Joback Method
dvisc	0.0006960	Pa×s	353.06	Joback Method
dvisc	0.0010392	Pa×s	318.15	Joback Method
dvisc	0.0017126	Pa×s	283.25	Joback Method
dvisc	0.0003018	Pa×s	457.78	Joback Method
dvisc	0.0032481	Pa×s	248.34	Joback Method
pvap	0.22	kPa	328.10	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.29	kPa	332.10	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furanaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol

pvap	0.40	kPa	338.00	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.55	kPa	343.00	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.15	kPa	323.00	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.08	kPa	313.70	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.05	kPa	308.20	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol

pvap	0.04	kPa	303.10	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.02	kPa	298.10	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.02	kPa	293.20	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol
pvap	0.11	kPa	317.90	Vapor Pressures, Enthalpies of Vaporization, and Limiting Activity Coefficients in Water at 100 deg C of 2-Furaldehyde, Benzaldehyde, Phenylethanal, and 2-Phenylethanol

Sources

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=C122781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Vapor Pressures, Enthalpies of
Vaporization, and Limiting Activity
Coefficients of Hexanal, Benzaldehyde,
2-Furalal, 2-Phenylbenzaldehyde,
Phenylethanal, and 2-Propylacetal
Water at Temperatures between (50 and
100) deg C:

<https://www.doi.org/10.1021/je060406c>

<https://www.doi.org/10.1021/je700122y>

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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

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