Benzeneacetaldehyde, «alpha»-methyl-

Other names:	(.+/-.)-Hydratropic aldehyde
	2-Fenyl-1-propanal
	2-Phenyl-1-propanal
	2-phenylpropanal
	2-phenylpropionaldehyde
	Aldehyd hydratropovy
	Benzene, (1-formylethyl)-
	Cumene aldehyde
	Hyacinthal
	Hydratropa aldehyde
	Hydratropaldehyde
	Hydratropic aldehyde
	Hydrotropic aldehyde
	NSC 5231
	Propionaldehyde, 2-phenyl-
	propanal, 2-phenyl-
	«alpha»-Formylethylbenzene
	«alpha»-Methyl-«alpha»-toluic aldehyde
	«alpha»-Methylphenylacetaldehyde
	«alpha»-Phenylpropionaldehyde
	«alpha»-Tolualdehyde, «alpha»-methyl-
Inchi:	InChI=1S/C9H10O/c1-8(7-10)9-5-3-2-4-6-9/h2-8H,1H3
InchiKey:	IQVAERDLDAZARL-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC(C=O)c1ccccc1
Mol. weight [g/mol]:	134.18
CAS:	93-53-8

Physical Properties

Property code	Value	Unit	Source
gf	35.35	kJ/mol	Joback Method
hf	-83.42	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	44.24	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.989		Crippen Method

mcvol	115.480	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	1083.90		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1093.60		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1093.60		NIST Webbook
rinpol	1083.90		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1612.00		NIST Webbook
tb	475.50 ± 1.50	K	NIST Webbook
tc	697.92	K	Joback Method
tf	244.61	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.06	J/mol×K	480.22	Joback Method
cpg	248.02	J/mol×K	516.50	Joback Method
cpg	260.17	J/mol×K	552.79	Joback Method
cpg	271.54	J/mol×K	589.07	Joback Method
cpg	282.17	J/mol×K	625.36	Joback Method
cpg	292.08	J/mol×K	661.64	Joback Method
cpg	301.32	J/mol×K	697.92	Joback Method
dvisc	0.0002787	Pa×s	480.22	Joback Method
dvisc	0.0021603	Pa×s	283.88	Joback Method
dvisc	0.0011754	Pa×s	323.15	Joback Method
dvisc	0.0048271	Pa×s	244.61	Joback Method
dvisc	0.0004973	Pa×s	401.68	Joback Method
dvisc	0.0003628	Pa×s	440.95	Joback Method
dvisc	0.0007297	Pa×s	362.41	Joback Method
hvapt	52.30 ± 0.20	kJ/mol	440.50	NIST Webbook
hvapt	49.40 ± 0.20	kJ/mol	440.50	NIST Webbook
hvapt	46.60 ± 0.30	kJ/mol	440.50	NIST Webbook
hvapt	43.40 ± 0.50	kJ/mol	440.50	NIST Webbook

pvap	3.06	kPa	373.10	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
pvap	20.97	kPa	423.15	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid:	https://www.doi.org/10.1021/je050327l
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=C93538&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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