Benzeneacetaldehyde, «alpha»-ethylidene-

Other names:	«alpha»-Ethylidenbenzeneacetaldehyde
	«alpha»-Ethylidenebenzeneacetaldehyde
	«alpha»-Ethylidene-phenylacetaldehyde
	2-Butenal, 2-phenyl
	2-Phenyl-2-buten-1-al
	2-Phenyl-2-butenal
	2-Phenylacetaldehyde, «alpha»-ethylidene
	2-Phenylbut-2-enal
	Benzeneacetaldehyde, a-ethylidene-
	2-phenylcrotonaldehyde
Inchi:	InChI=1S/C10H10O/c1-2-9(8-11)10-6-4-3-5-7-10/h2-8H,1H3/b9-2+
InchiKey:	DYAOGZLLMZQVHY-XNWCZRBMSA-N
Formula:	C10H10O
SMILES:	CC=C(C=O)c1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	4411-89-6

Physical Properties

Property code	Value	Unit	Source
gf	117.88	kJ/mol	Joback Method
hf	8.65	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.289		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1283.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1265.00		NIST Webbook

rinpol	1273.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1274.40		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1232.00		NIST Webbook
ripol	1972.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1911.00		NIST Webbook
ripol	1913.00		NIST Webbook
ripol	1922.00		NIST Webbook
ripol	1922.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1939.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	507.58	K	Joback Method
tc	731.50	K	Joback Method
tf	251.84	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.82	J/mol×K	507.58	Joback Method
cpg	273.09	J/mol×K	544.90	Joback Method
cpg	285.43	J/mol×K	582.22	Joback Method
cpg	296.89	J/mol×K	619.54	Joback Method
cpg	307.53	J/mol×K	656.86	Joback Method
cpg	317.40	J/mol×K	694.18	Joback Method
cpg	326.56	J/mol×K	731.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4411896&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
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