

2-Phenylpropenal

Other names:	Benzeneacetaldehyde, «alpha»-methylene-Atropaldehyde «alpha»-Phenylacrolein 2-phenyl-2-propenal
Inchi:	InChI=1S/C9H8O/c1-8(7-10)9-5-3-2-4-6-9/h2-7H,1H2
InchiKey:	ZFBRJUBOJXNIQM-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	<chem>C=C(C=O)c1ccccc1</chem>
Mol. weight [g/mol]:	132.16
CAS:	4432-63-7

Physical Properties

Property code	Value	Unit	Source
gf	117.08	kJ/mol	Joback Method
hf	37.50	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	44.03	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.899		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1147.60		NIST Webbook
rinpol	1147.60		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	477.22	K	Joback Method
tc	699.09	K	Joback Method
tf	243.89	K	Joback Method
vc	0.430	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.66	J/mol×K	477.22	Joback Method
cpg	229.71	J/mol×K	514.20	Joback Method
cpg	240.92	J/mol×K	551.18	Joback Method
cpg	251.36	J/mol×K	588.15	Joback Method
cpg	261.05	J/mol×K	625.13	Joback Method
cpg	270.05	J/mol×K	662.11	Joback Method
cpg	278.39	J/mol×K	699.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4432637&Units=SI

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
ripol:	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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