

1,3-Dioxolane, 2-phenyl-

Other names:	Benzaldehyde ethylene acetal 2-Phenyl-1,3-dioxolane
Inchi:	InChI=1S/C9H10O2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-5,9H,6-7H2
InchiKey:	LYINTWKRUWVLBA-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	c1ccc(C2OCCO2)cc1
Mol. weight [g/mol]:	150.17
CAS:	936-51-6

Physical Properties

Property code	Value	Unit	Source
chl	-4703.30	kJ/mol	NIST Webbook
gf	1.62	kJ/mol	Joback Method
hf	-205.30 ± 1.30	kJ/mol	NIST Webbook
hfl	-267.40 ± 1.30	kJ/mol	NIST Webbook
hfus	23.00	kJ/mol	Joback Method
hvap	62.10	kJ/mol	NIST Webbook
hvap	62.13 ± 0.25	kJ/mol	NIST Webbook
hvap	62.60 ± 0.70	kJ/mol	NIST Webbook
log10ws	-1.72		Crippen Method
logp	1.732		Crippen Method
mcvol	114.790	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	413.20	K	NIST Webbook
tc	741.52	K	Joback Method
tf	281.65	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	336.95	J/molxK	741.52	Joback Method
cpg	257.04	J/molxK	501.18	Joback Method
cpg	273.09	J/molxK	541.24	Joback Method
cpg	287.97	J/molxK	581.29	Joback Method
cpg	301.75	J/molxK	621.35	Joback Method
cpg	314.46	J/molxK	661.41	Joback Method
cpg	326.18	J/molxK	701.46	Joback Method
dvisc	0.0003581	Paxs	501.18	Joback Method
dvisc	0.0040267	Paxs	281.65	Joback Method
dvisc	0.0021336	Paxs	318.24	Joback Method
dvisc	0.0012887	Paxs	354.83	Joback Method
dvisc	0.0008553	Paxs	391.41	Joback Method
dvisc	0.0006089	Paxs	428.00	Joback Method
dvisc	0.0004573	Paxs	464.59	Joback Method
hvapt	62.10 ± 0.30	kJ/mol	315.50	NIST Webbook

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=C936516&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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