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	62.13 ± 0.25	kJ/mol	NIST Webbook
hvap	62.10	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	336.95	J/mol×K	741.52	Joback Method
cpg	257.04	J/mol×K	501.18	Joback Method
cpg	273.09	J/mol×K	541.24	Joback Method
cpg	287.97	J/mol×K	581.29	Joback Method
cpg	301.75	J/mol×K	621.35	Joback Method
cpg	314.46	J/mol×K	661.41	Joback Method
cpg	326.18	J/mol×K	701.46	Joback Method
dvisc	0.0003581	Pa×s	501.18	Joback Method
dvisc	0.0040267	Pa×s	281.65	Joback Method
dvisc	0.0021336	Pa×s	318.24	Joback Method
dvisc	0.0012887	Pa×s	354.83	Joback Method
dvisc	0.0008553	Pa×s	391.41	Joback Method
dvisc	0.0006089	Pa×s	428.00	Joback Method
dvisc	0.0004573	Pa×s	464.59	Joback Method
hvapt	62.10 ± 0.30	kJ/mol	315.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C936516&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

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