1,3-Dioxolane, 2-(2-phenylethenyl), (Z)

Inchi: InChI=1S/C11H12O2/c1-2-4-10(5-3-1)6-7-11-12-8-9-13-11/h1-7,11H,8-9H2/b7-6-
InchiKey: JQLASNFFJHGQTK-SREVYHEPSA-N
Formula: C11H12O2
SMILES: C(=CC1OCCO1)c1ccccc1
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
gf	98.68	kJ/mol	Joback Method
hf	-120.14	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.073		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1503.00		NIST Webbook
tb	551.10	K	Joback Method
tc	793.42	K	Joback Method
tf	299.11	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.01	J/mol×K	551.10	Joback Method
cpg	347.14	J/mol×K	591.49	Joback Method
cpg	362.94	J/mol×K	631.87	Joback Method
cpg	377.50	J/mol×K	672.26	Joback Method
cpg	390.89	J/mol×K	712.65	Joback Method
cpg	403.20	J/mol×K	753.04	Joback Method
cpg	414.52	J/mol×K	793.42	Joback Method
dvisc	0.0036566	Pa×s	299.11	Joback Method
dvisc	0.0018009	Pa×s	341.11	Joback Method

dvisc	0.0010360	Pa×s	383.11	Joback Method
dvisc	0.0006648	Pa×s	425.11	Joback Method
dvisc	0.0004620	Pa×s	467.10	Joback Method
dvisc	0.0003409	Pa×s	509.10	Joback Method
dvisc	0.0002635	Pa×s	551.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329401&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

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
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