

1,3-Dioxolane, 2-ethyl-4-phenyl, # 1

Inchi:	InChI=1S/C11H14O2/c1-2-11-12-8-10(13-11)9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3
InchiKey:	YK GKRD IKD NYZNF-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCC1OCC(c2ccccc2)O1
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
gf	10.75	kJ/mol	Joback Method
hf	-257.70	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.511		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1871.00		NIST Webbook
tb	542.27	K	Joback Method
tc	773.49	K	Joback Method
tf	299.95	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.88	J/molxK	542.27	Joback Method
cpg	428.95	J/molxK	734.95	Joback Method
cpg	415.37	J/molxK	696.42	Joback Method
cpg	400.72	J/molxK	657.88	Joback Method
cpg	384.95	J/molxK	619.34	Joback Method
cpg	368.02	J/molxK	580.81	Joback Method

cpg	441.52	J/molxK	773.49	Joback Method
dvisc	0.0003432	Paxs	542.27	Joback Method
dvisc	0.0004286	Paxs	501.88	Joback Method
dvisc	0.0005564	Paxs	461.50	Joback Method
dvisc	0.0007593	Paxs	421.11	Joback Method
dvisc	0.0011070	Paxs	380.72	Joback Method
dvisc	0.0017650	Paxs	340.34	Joback Method
dvisc	0.0031907	Paxs	299.95	Joback Method

Sources

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=R409191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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