Acetone-1-phenyl 1,2-ethandiol ketal

Other names: 1,3-Dioxolane, 2,2-dimethyl-4-phenyl
Inchi: InChI=1S/C11H14O2/c1-11(2)12-8-10(13-11)9-6-4-3-5-7-9/h3-7,10H,8H2,1-2H3
InchiKey: SFDXYHMRHIVYET-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC1(C)OCC(c2ccccc2)O1
Mol. weight [g/mol]: 178.23
CAS: 52129-03-0

Physical Properties

Property code	Value	Unit	Source
gf	5.26	kJ/mol	Joback Method
hf	-242.46	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.511		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
ripol	1766.00		NIST Webbook
tb	542.51	K	Joback Method
tc	783.75	K	Joback Method
tf	323.85	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.20	J/mol×K	542.51	Joback Method
cpg	367.12	J/mol×K	582.72	Joback Method
cpg	383.68	J/mol×K	622.92	Joback Method
cpg	399.06	J/mol×K	663.13	Joback Method
cpg	413.43	J/mol×K	703.34	Joback Method

cpg	426.95	J/mol×K	743.54	Joback Method
cpg	439.81	J/mol×K	783.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52129030&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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