1,2,4-Trioxolane, 3,5-diphenyl-

Other names: Benzene, 1,1'-(1,2-ethenediyl)bis-, ozonide
3,5-diphenyl-1,2,4-trioxolane
Inchi: InChI=1S/C14H12O3/c1-3-7-11(8-4-1)13-15-14(17-16-13)12-9-5-2-6-10-12/h1-10,13-14H
InchiKey: FFNQUPJQBYSJAG-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: c1ccc(C2OOC(c3ccccc3)O2)cc1
Mol. weight [g/mol]: 228.24
CAS: 23888-15-5

Physical Properties

Property code	Value	Unit	Source
chs	-7100.00 ± 8.00	kJ/mol	NIST Webbook
gf	62.30	kJ/mol	Joback Method
hf	-215.09	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.362		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	664.54	K	Joback Method
tc	928.62	K	Joback Method
tf	386.75	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.67	J/mol×K	664.54	Joback Method
cpg	527.91	J/mol×K	884.61	Joback Method
cpg	516.15	J/mol×K	840.60	Joback Method
cpg	503.04	J/mol×K	796.58	Joback Method
cpg	488.49	J/mol×K	752.57	Joback Method
cpg	472.40	J/mol×K	708.55	Joback Method

cpg	538.42	J/mol×K	928.62	Joback Method
dvisc	0.0002598	Pa×s	664.54	Joback Method
dvisc	0.0003269	Pa×s	618.24	Joback Method
dvisc	0.0004269	Pa×s	571.94	Joback Method
dvisc	0.0005844	Pa×s	525.64	Joback Method
dvisc	0.0008501	Pa×s	479.35	Joback Method
dvisc	0.0013397	Pa×s	433.05	Joback Method
dvisc	0.0023542	Pa×s	386.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23888155&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

chs:	Standard solid 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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