1,3-Diphenyl-2,3-epoxy-1-propanone

Other names:	Chalcone trans-«alpha»,«beta»-epoxide
	Chalcone-«alpha»,«beta»-epoxide
	Methanone, phenyl(3-phenyloxiranyl)-
	phenyl (3-phenyloxiranyl) ketone
Inchi:	InChI=1S/C15H12O2/c16-13(11-7-3-1-4-8-11)15-14(17-15)12-9-5-2-6-10-12/h1-10,14-15
InchiKey:	UQGMJZQVDNZRKT-UHFFFAOYSA-N
Formula:	C15H12O2
SMILES:	O=C(c1ccccc1)C1OC1c1ccccc1
Mol. weight [g/mol]:	224.25
CAS:	5411-12-1

Physical Properties

Property code	Value	Unit	Source
chs	-7522.00	kJ/mol	NIST Webbook
gf	138.24	kJ/mol	Joback Method
hf	-71.99	kJ/mol	Joback Method
hfs	-128.00	kJ/mol	NIST Webbook
hfus	31.47	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.009		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	678.85	K	Joback Method
tc	933.79	K	Joback Method
tf	401.85	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.27	J/mol×K	678.85	Joback Method
cpg	474.52	J/mol×K	721.34	Joback Method
cpg	489.32	J/mol×K	763.83	Joback Method

cpg	502.81	J/mol×K	806.32	Joback Method
cpg	515.10	J/mol×K	848.81	Joback Method
cpg	526.33	J/mol×K	891.30	Joback Method
cpg	536.62	J/mol×K	933.79	Joback Method
dvisc	0.0023451	Pa×s	401.85	Joback Method
dvisc	0.0015966	Pa×s	448.02	Joback Method
dvisc	0.0011680	Pa×s	494.18	Joback Method
dvisc	0.0009013	Pa×s	540.35	Joback Method
dvisc	0.0007245	Pa×s	586.52	Joback Method
dvisc	0.0006012	Pa×s	632.68	Joback Method
dvisc	0.0005117	Pa×s	678.85	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5411121&Units=SI

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
hfs: Solid phase 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