

1,2-Indandiol, diacetate, cis-

Inchi:	InChI=1S/C13H14O4/c1-8(14)16-12-7-10-5-3-4-6-11(10)13(12)17-9(2)15/h3-6,12-13H,7H
InchiKey:	ZSAGZMJOVRIXMF-OLZOCXBDSA-N
Formula:	C13H14O4
SMILES:	CC(=O)OC1Cc2ccccc2C1OC(C)=O
Mol. weight [g/mol]:	234.25
CAS:	19597-96-7

Physical Properties

Property code	Value	Unit	Source
chs	-6341.70	kJ/mol	NIST Webbook
gf	-253.44	kJ/mol	Joback Method
hf	-523.73	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.779		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	683.15	K	Joback Method
tc	905.01	K	Joback Method
tf	433.23	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.86	J/molxK	683.15	Joback Method
cpg	538.35	J/molxK	868.03	Joback Method
cpg	527.54	J/molxK	831.06	Joback Method
cpg	515.81	J/molxK	794.08	Joback Method
cpg	503.14	J/molxK	757.10	Joback Method
cpg	489.50	J/molxK	720.13	Joback Method
cpg	548.27	J/molxK	905.01	Joback Method
dvisc	0.0004286	Paxs	683.15	Joback Method

dvisc	0.0004938	Paxs	641.50	Joback Method
dvisc	0.0005802	Paxs	599.84	Joback Method
dvisc	0.0006984	Paxs	558.19	Joback Method
dvisc	0.0008660	Paxs	516.54	Joback Method
dvisc	0.0011153	Paxs	474.88	Joback Method
dvisc	0.0015080	Paxs	433.23	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=C19597967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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