cis-Indan-1,2-diol, diacetate

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

Physical Properties

Property code	Value	Unit	Source
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
rinpol	1610.00		NIST Webbook
tb	683.15	K	Joback Method
tc	905.01	K	Joback Method
tf	433.23	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.86	J/mol×K	683.15	Joback Method
cpg	489.50	J/mol×K	720.13	Joback Method
cpg	503.14	J/mol×K	757.10	Joback Method
cpg	515.81	J/mol×K	794.08	Joback Method
cpg	527.54	J/mol×K	831.06	Joback Method
cpg	538.35	J/mol×K	868.03	Joback Method
cpg	548.27	J/mol×K	905.01	Joback Method
dvisc	0.0015080	Pa×s	433.23	Joback Method
dvisc	0.0011153	Pa×s	474.88	Joback Method

dvisc	0.0008660	Pa×s	516.54	Joback Method
dvisc	0.0006984	Pa×s	558.19	Joback Method
dvisc	0.0005802	Pa×s	599.84	Joback Method
dvisc	0.0004938	Pa×s	641.50	Joback Method
dvisc	0.0004286	Pa×s	683.15	Joback Method

Sources

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=R109381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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