trans-Indan-1,2-diol, diacetate

Inchi: InChI=1S/C13H16O4/c1-8(14)16-12-7-10-5-3-4-6-11(10)13(12)17-9(2)15/h3-6,10-13H,7H
InchiKey: ZIRUILRHTIAUOR-TYUFSLCMSA-N
Formula: C13H16O4
SMILES: CC(=O)OC1CC2C=CC=CC2C1OC(C)=O
Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	-279.56	kJ/mol	Joback Method
hf	-599.25	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.612		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1610.00		NIST Webbook
tb	664.69	K	Joback Method
tc	883.02	K	Joback Method
tf	398.95	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.69	J/mol×K	664.69	Joback Method
cpg	578.63	J/mol×K	846.63	Joback Method
cpg	566.02	J/mol×K	810.24	Joback Method
cpg	552.34	J/mol×K	773.85	Joback Method
cpg	537.58	J/mol×K	737.47	Joback Method
cpg	521.70	J/mol×K	701.08	Joback Method
cpg	590.20	J/mol×K	883.02	Joback Method
dvisc	0.0005787	Pa×s	664.69	Joback Method
dvisc	0.0006577	Pa×s	620.40	Joback Method

dvisc	0.0007625	Pa×s	576.11	Joback Method
dvisc	0.0009059	Pa×s	531.82	Joback Method
dvisc	0.0011107	Pa×s	487.53	Joback Method
dvisc	0.0014182	Pa×s	443.24	Joback Method
dvisc	0.0019119	Pa×s	398.95	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109821&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
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