trans-Indan-1,2-diol

Inchi: InChI=1S/C9H12O2/c10-8-5-6-3-1-2-4-7(6)9(8)11/h1-4,6-11H,5H2/t6?,7?,8-,9-/m0/s1
InchiKey: WHWGIACBFRFQHW-PEBLOWIWSA-N
Formula: C9H12O2
SMILES: OC1CC2C=CC=CC2C1O
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
gf	-119.04	kJ/mol	Joback Method
hf	-331.55	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.470		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
rinpol	1440.00		NIST Webbook
tb	604.95	K	Joback Method
tc	798.19	K	Joback Method
tf	331.19	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.85	J/mol×K	604.95	Joback Method
cpg	341.09	J/mol×K	637.16	Joback Method
cpg	352.59	J/mol×K	669.36	Joback Method
cpg	363.39	J/mol×K	701.57	Joback Method
cpg	373.53	J/mol×K	733.78	Joback Method
cpg	383.04	J/mol×K	765.98	Joback Method
cpg	391.95	J/mol×K	798.19	Joback Method
dvisc	0.0139990	Pa×s	331.19	Joback Method
dvisc	0.0038674	Pa×s	376.82	Joback Method

dvisc	0.0014106	Pa×s	422.44	Joback Method
dvisc	0.0006263	Pa×s	468.07	Joback Method
dvisc	0.0003212	Pa×s	513.70	Joback Method
dvisc	0.0001837	Pa×s	559.32	Joback Method
dvisc	0.0001143	Pa×s	604.95	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=R109792&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