cis-Tetralin-1,2-diol, diacetate

Inchi: InChI=1S/C14H16O4/c1-9(15)17-13-8-7-11-5-3-4-6-12(11)14(13)18-10(2)16/h3-6,13-14H
InchiKey: PWDTYDXUIYVSGG-UONOGXRCSA-N
Formula: C14H16O4
SMILES: CC(=O)OC1CCc2ccccc2C1OC(C)=O
Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
gf	-257.12	kJ/mol	Joback Method
hf	-550.53	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	67.78	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.169		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	710.30	K	Joback Method
tc	934.93	K	Joback Method
tf	440.98	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.85	J/mol×K	710.30	Joback Method
cpg	545.60	J/mol×K	747.74	Joback Method
cpg	560.22	J/mol×K	785.18	Joback Method
cpg	573.73	J/mol×K	822.62	Joback Method
cpg	586.14	J/mol×K	860.06	Joback Method
cpg	597.49	J/mol×K	897.49	Joback Method
cpg	607.78	J/mol×K	934.93	Joback Method
dvisc	0.0013605	Pa×s	440.98	Joback Method

dvisc	0.0009336	Pa×s	485.87	Joback Method
dvisc	0.0006828	Pa×s	530.75	Joback Method
dvisc	0.0005244	Pa×s	575.64	Joback Method
dvisc	0.0004184	Pa×s	620.53	Joback Method
dvisc	0.0003441	Pa×s	665.41	Joback Method
dvisc	0.0002901	Pa×s	710.30	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=R109623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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