

trans-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-ZIAGYGMSSA-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	1705.00		NIST Webbook
rinpol	1705.00		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/molxK	710.30	Joback Method
cpg	545.60	J/molxK	747.74	Joback Method
cpg	560.22	J/molxK	785.18	Joback Method
cpg	573.73	J/molxK	822.62	Joback Method
cpg	586.14	J/molxK	860.06	Joback Method
cpg	597.49	J/molxK	897.49	Joback Method
cpg	607.78	J/molxK	934.93	Joback Method
dvisc	0.0013605	Paxs	440.98	Joback Method

dvisc	0.0009336	Paxs	485.87	Joback Method
dvisc	0.0006828	Paxs	530.75	Joback Method
dvisc	0.0005244	Paxs	575.64	Joback Method
dvisc	0.0004184	Paxs	620.53	Joback Method
dvisc	0.0003441	Paxs	665.41	Joback Method
dvisc	0.0002901	Paxs	710.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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