tyrosol acetate

Inchi: InChI=1S/C12H14O4/c1-9(13)15-8-7-11-3-5-12(6-4-11)16-10(2)14/h3-6H,7-8H2,1-2H3
InchiKey: JRBAXMAMWTZVRE-UHFFFAOYSA-N
Formula: C12H14O4
SMILES: CC(=O)OCCc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	-314.90	kJ/mol	Joback Method
hf	-555.55	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.717		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	658.20	K	Joback Method
tc	870.02	K	Joback Method
tf	408.26	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/mol×K	658.20	Joback Method
cpg	449.86	J/mol×K	693.50	Joback Method
cpg	462.40	J/mol×K	728.81	Joback Method
cpg	474.13	J/mol×K	764.11	Joback Method
cpg	485.06	J/mol×K	799.41	Joback Method
cpg	495.18	J/mol×K	834.72	Joback Method
cpg	504.49	J/mol×K	870.02	Joback Method
dvisc	0.0011118	Pa×s	408.26	Joback Method

dvisc	0.0006814	Pa×s	449.92	Joback Method
dvisc	0.0004537	Pa×s	491.57	Joback Method
dvisc	0.0003219	Pa×s	533.23	Joback Method
dvisc	0.0002401	Pa×s	574.89	Joback Method
dvisc	0.0001863	Pa×s	616.54	Joback Method
dvisc	0.0001492	Pa×s	658.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490850&Units=SI

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