Eriodictyol

Inchi: InChI=1S/C15H12O6/c16-8-4-11(19)15-12(20)6-13(21-14(15)5-8)7-1-2-9(17)10(18)3-7/h
InchiKey: SBHXYTNGIZCORC-UHFFFAOYSA-N
Formula: C15H12O6
SMILES: O=C1CC(c2ccc(O)c(O)c2)Oc2cc(O)cc(O)c21
Mol. weight [g/mol]: 288.25

Physical Properties

Property code	Value	Unit	Source
gf	-487.93	kJ/mol	Joback Method
hf	-803.64	kJ/mol	Joback Method
hfus	48.95	kJ/mol	Joback Method
hvap	115.10	kJ/mol	Joback Method
log10ws	-3.62		Aqueous Solubility Prediction Method
log10ws	-3.62		Estimated Solubility Method
logp	2.215		Crippen Method
mcvol	194.750	ml/mol	McGowan Method
pc	6567.04	kPa	Joback Method
tb	1029.20	K	Joback Method
tc	1315.14	K	Joback Method
tf	880.26	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.80	J/mol×K	1029.20	Joback Method
cpg	672.85	J/mol×K	1076.86	Joback Method
cpg	693.92	J/mol×K	1124.51	Joback Method
cpg	717.46	J/mol×K	1172.17	Joback Method
cpg	743.90	J/mol×K	1219.82	Joback Method
cpg	773.69	J/mol×K	1267.48	Joback Method
cpg	807.25	J/mol×K	1315.14	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume