hematein

Inchi: InChI=1S/C16H12O6/c17-10-2-1-8-13-9-4-12(19)11(18)3-7(9)5-16(13,21)6-22-15(8)14(1
InchiKey: HLUCICHZHWJHLL-UHFFFAOYSA-N
Formula: C16H12O6
SMILES: O=C1C=C2CC3(O)COc4c(ccc(O)c4O)C3=C2C=C1O
Mol. weight [g/mol]: 300.27

Physical Properties

Property code	Value	Unit	Source
gf	-385.63	kJ/mol	Joback Method
hf	-687.83	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	125.36	kJ/mol	Joback Method
log10ws	-2.70		Estimated Solubility Method
log10ws	-2.70		Aqueous Solubility Prediction Method
logp	1.330		Crippen Method
mcvol	197.980	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
tb	1093.25	K	Joback Method
tc	1348.15	K	Joback Method
tf	880.41	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.86	J/mol×K	1093.25	Joback Method
cpg	727.41	J/mol×K	1135.73	Joback Method
cpg	756.08	J/mol×K	1178.22	Joback Method
cpg	788.26	J/mol×K	1220.70	Joback Method
cpg	824.33	J/mol×K	1263.19	Joback Method
cpg	864.69	J/mol×K	1305.67	Joback Method
cpg	909.73	J/mol×K	1348.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

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