prostaglandin E2

Inchi: InChI=1S/C20H32O5/c1-2-3-6-9-15(21)12-13-17-16(18(22)14-19(17)23)10-7-4-5-8-11-20
InchiKey: XEYBRNLFEZDVAW-UHFFFAOYSA-N
Formula: C20H32O5
SMILES: CCCCCC(O)C=CC1C(O)CC(=O)C1CC=CCCCC(=O)O
Mol. weight [g/mol]: 352.47

Physical Properties

Property code	Value	Unit	Source
gf	-365.32	kJ/mol	Joback Method
hf	-914.14	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	120.31	kJ/mol	Joback Method
log10ws	-2.47		Aqueous Solubility Prediction Method
logp	3.251		Crippen Method
mcvol	293.950	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
tb	1069.05	K	Joback Method
tc	1320.80	K	Joback Method
tf	593.03	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.46	J/mol×K	1069.05	Joback Method
cpg	1071.46	J/mol×K	1111.01	Joback Method
cpg	1084.14	J/mol×K	1152.97	Joback Method
cpg	1095.59	J/mol×K	1194.93	Joback Method
cpg	1105.91	J/mol×K	1236.89	Joback Method
cpg	1115.19	J/mol×K	1278.85	Joback Method
cpg	1123.52	J/mol×K	1320.80	Joback Method

Sources

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

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