Benzofuran deriv (herz)

Inchi: InChI=1S/C14H16O4/c1-7(2)11-6-9-5-10(8(3)15)12(16)14(17-4)13(9)18-11/h5,11,16H,1,
InchiKey: IRBPQIXYOCSHLL-UHFFFAOYSA-N
Formula: C14H16O4
SMILES: C=C(C)C1Cc2cc(C(C)=O)c(O)c(OC)c2O1
Mol. weight [g/mol]: 248.27
CAS: 35817-13-1

Physical Properties

Property code	Value	Unit	Source
gf	-184.10	kJ/mol	Joback Method
hf	-495.84	kJ/mol	Joback Method
hfus	36.98	kJ/mol	Joback Method
hvap	77.02	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.483		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	748.50	K	Joback Method
tc	977.90	K	Joback Method
tf	524.19	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.14	J/mol×K	748.50	Joback Method
cpg	550.54	J/mol×K	786.73	Joback Method
cpg	563.19	J/mol×K	824.97	Joback Method
cpg	575.20	J/mol×K	863.20	Joback Method
cpg	586.67	J/mol×K	901.44	Joback Method
cpg	597.68	J/mol×K	939.67	Joback Method
cpg	608.34	J/mol×K	977.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.00	K	0.07	NIST Webbook

Sources

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=C35817131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume