Alpha-benzamido-4-hydroxy-3,5-diiodohydrocinna

Inchi: InChI=1S/C16H14I2N2O3/c17-11-6-9(7-12(18)14(11)21)8-13(15(19)22)20-16(23)10-4-2-
InchiKey: QJPXSFLBPXVGFN-UHFFFAOYSA-N
Formula: C16H14I2N2O3
SMILES: NC(=O)C(Cc1cc(I)c(O)c(I)c1)NC(=O)c1ccccc1
Mol. weight [g/mol]: 536.10
CAS: 195067-02-8

Physical Properties

Property code	Value	Unit	Source
gf	146.58	kJ/mol	Joback Method
hf	-90.20	kJ/mol	Joback Method
hfus	49.07	kJ/mol	Joback Method
hvap	119.03	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	2.428		Crippen Method
mcvol	269.390	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
tb	1125.70	K	Joback Method
tc	1417.69	K	Joback Method
tf	796.58	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.38	J/mol×K	1125.70	Joback Method
cpg	738.06	J/mol×K	1174.37	Joback Method
cpg	751.42	J/mol×K	1223.03	Joback Method
cpg	765.73	J/mol×K	1271.70	Joback Method
cpg	781.28	J/mol×K	1320.36	Joback Method
cpg	798.33	J/mol×K	1369.03	Joback Method
cpg	817.16	J/mol×K	1417.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C195067028&Units=SI
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

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